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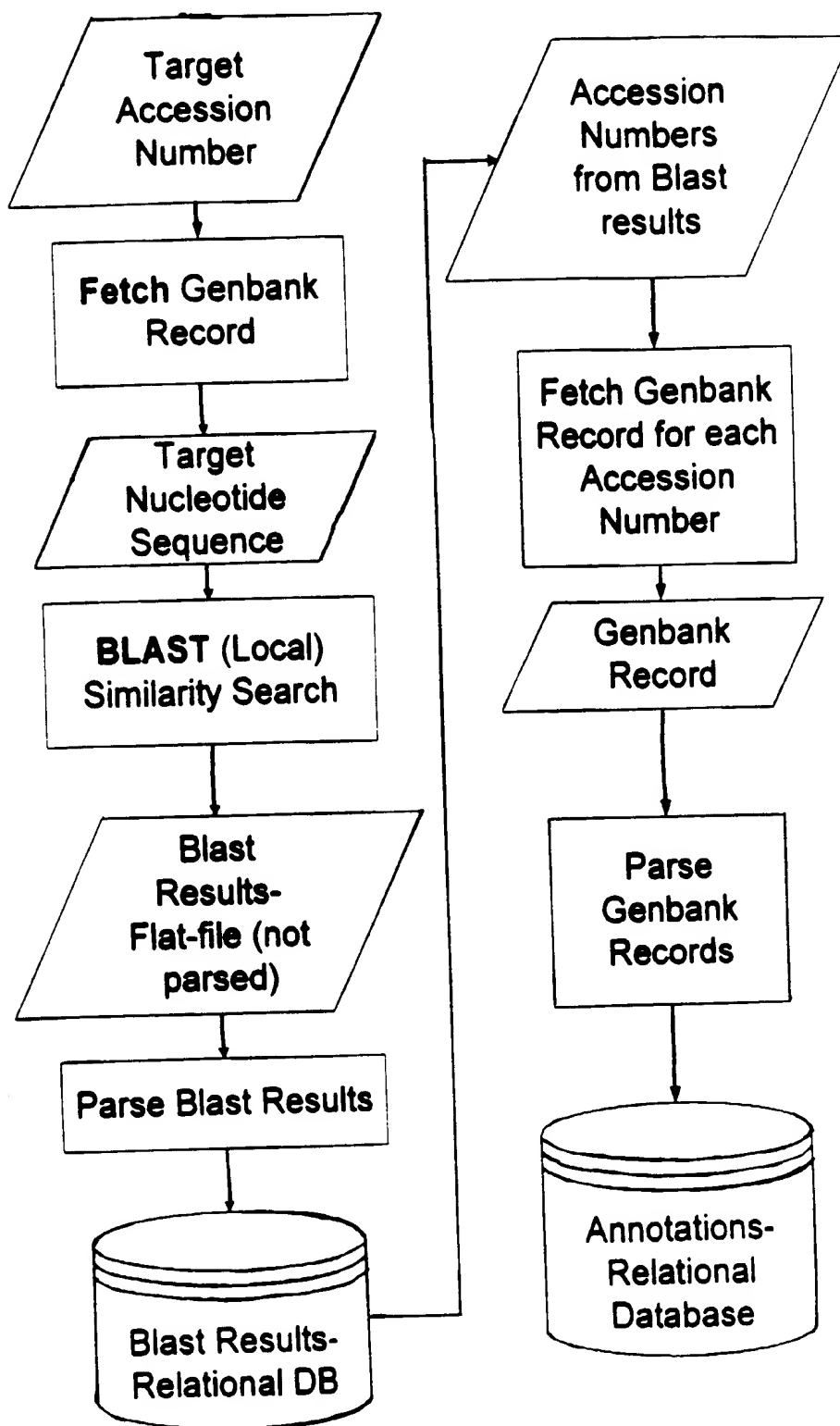


Figure 3

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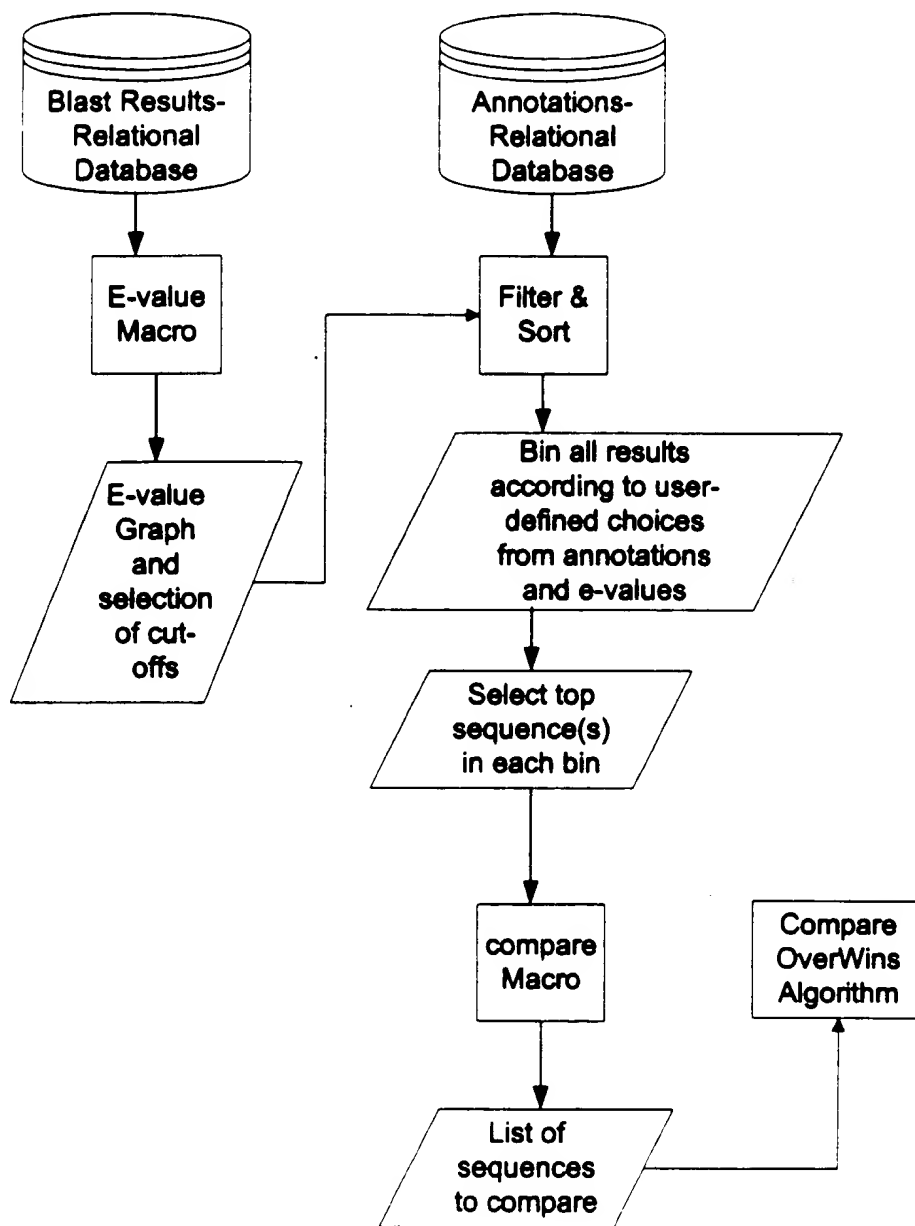


FIGURE 4

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CompareOverWins
Algorithm Flow Chart

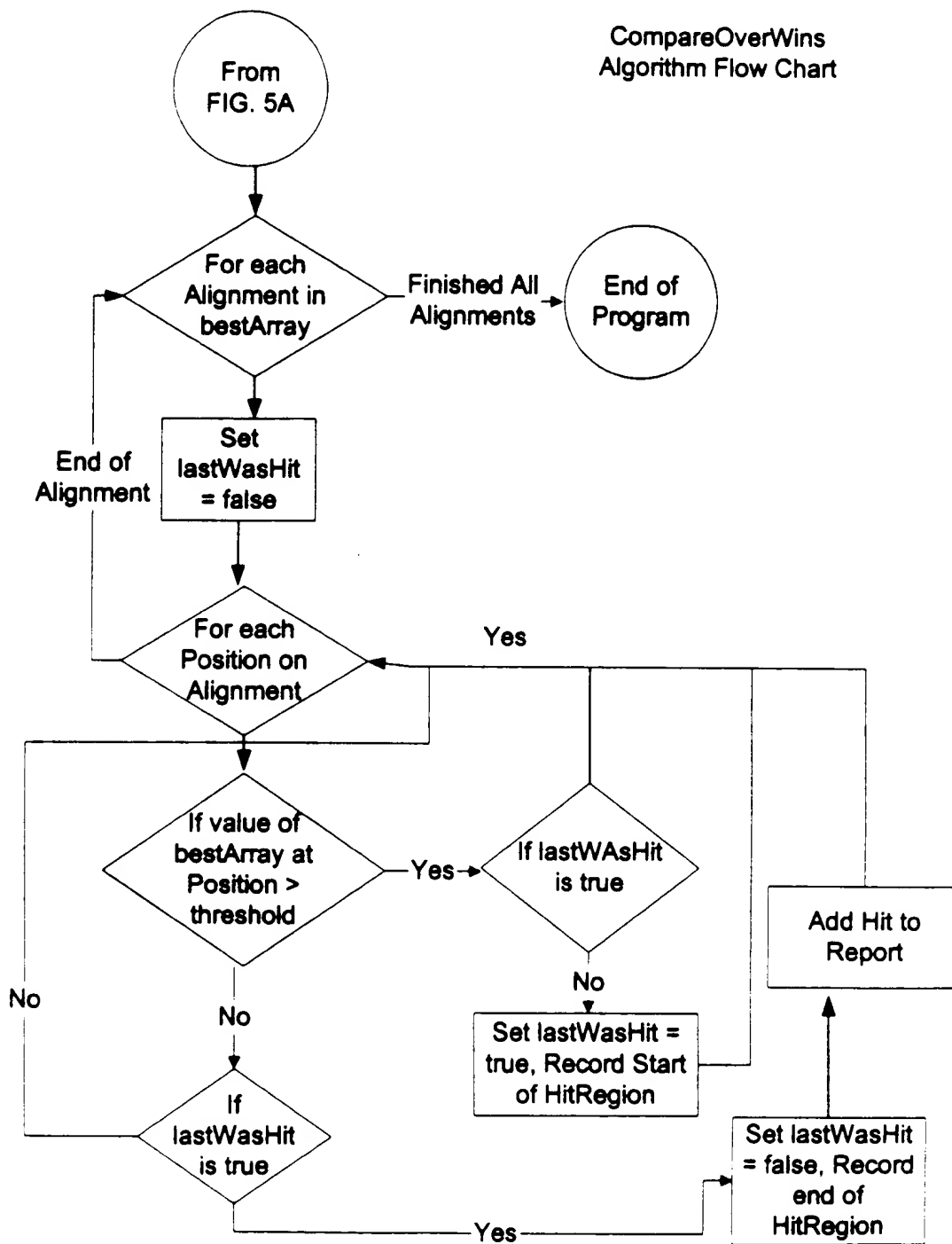


FIGURE 5B

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**CompareOverWins
 Algorithm Flow Chart
 Basic Compare**

Input:
 Sequence A length a
 Sequence B length b
 Window Size

Output:
 Array of size a by b of unsigned chars (0-255)
 Each point represents the number of matches in the
 window at that alignment and position

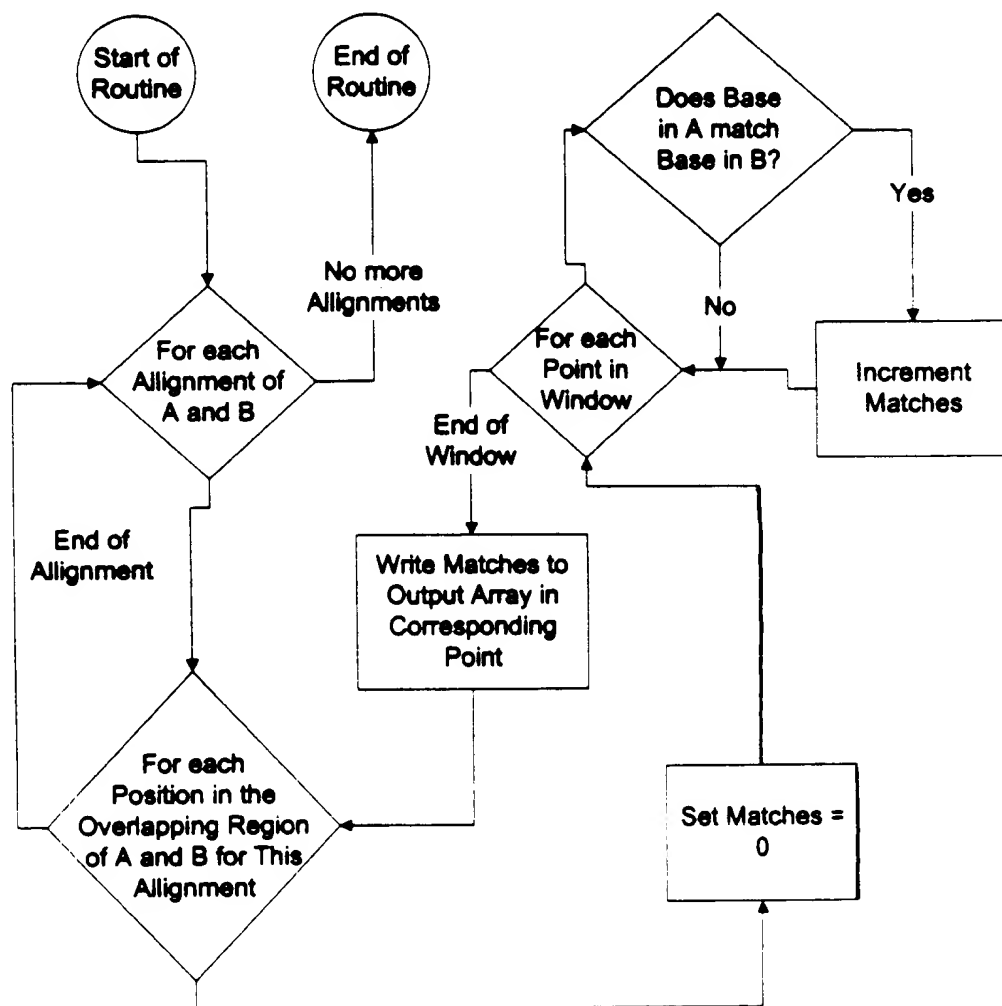
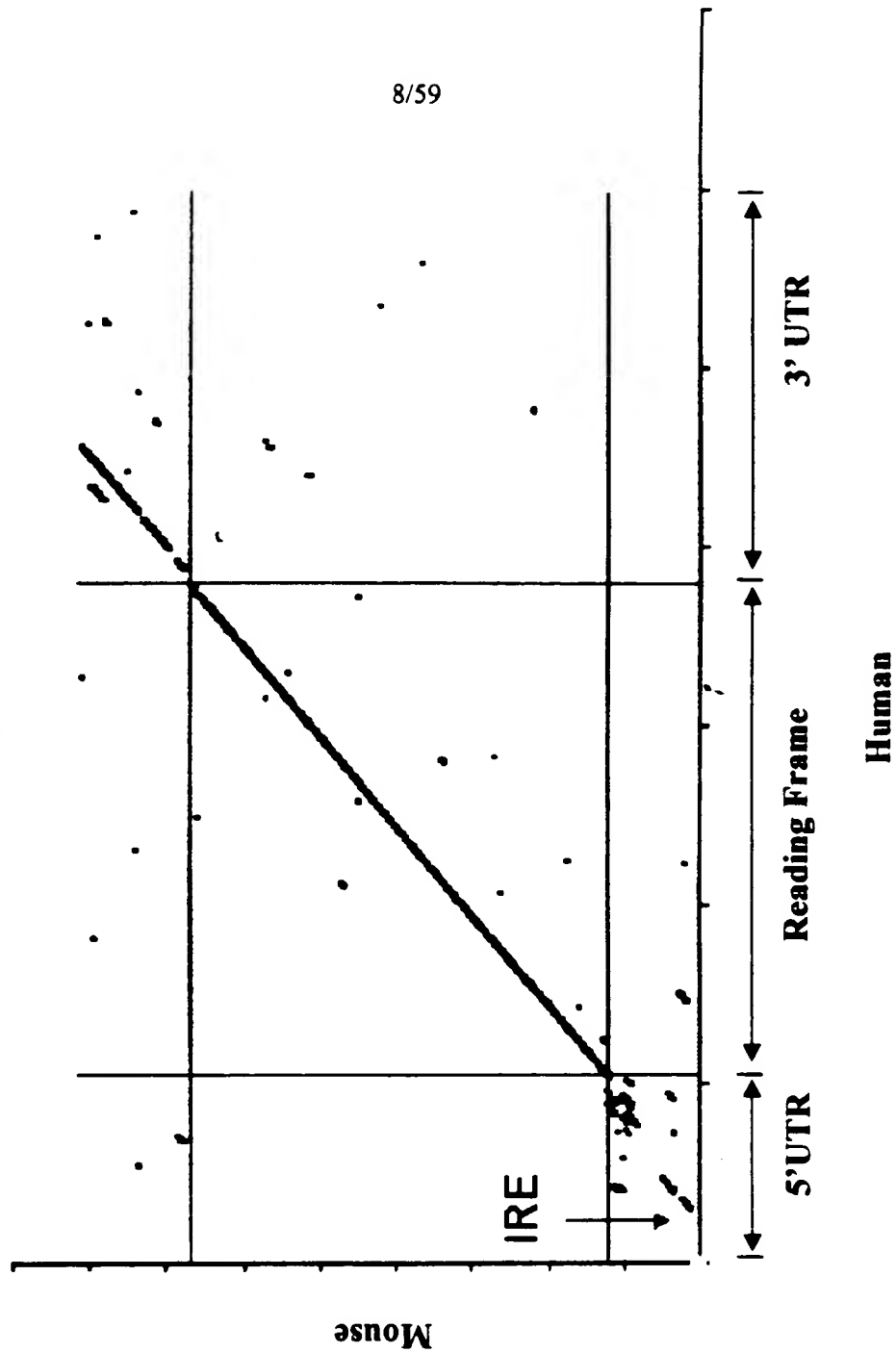


FIGURE 5C

Figure 6



Self Complementation Analysis - Single Sequence

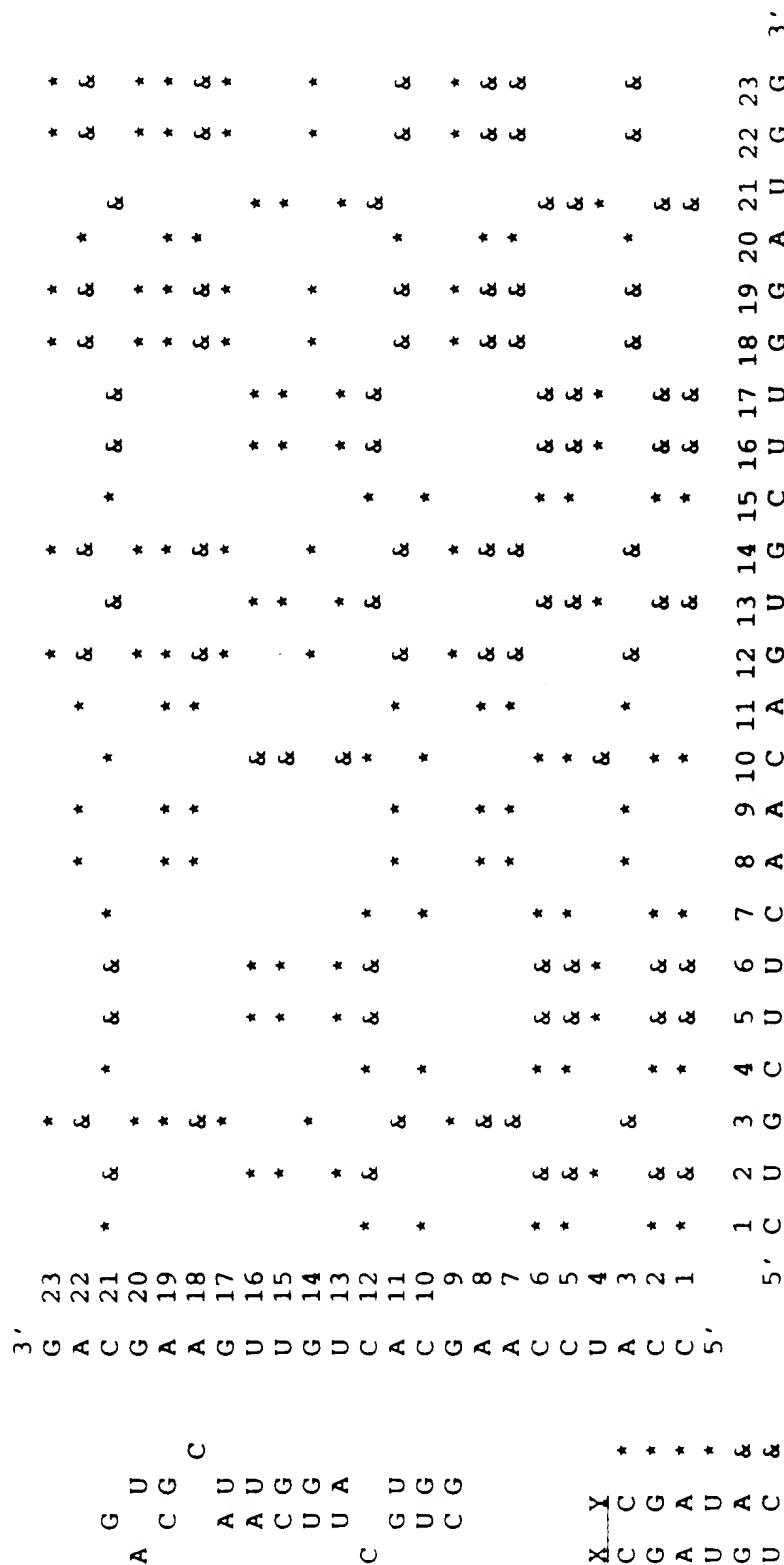
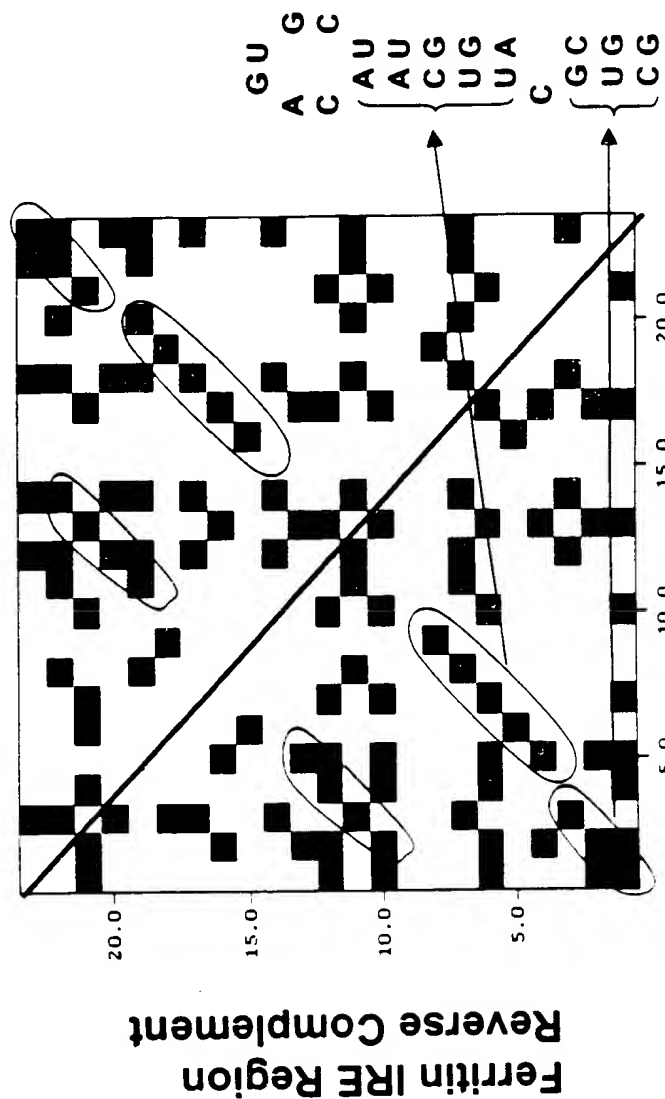


Figure 7

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Self Complementarity Comparisons

13 ortholog overlay



Ferritin IRE Region

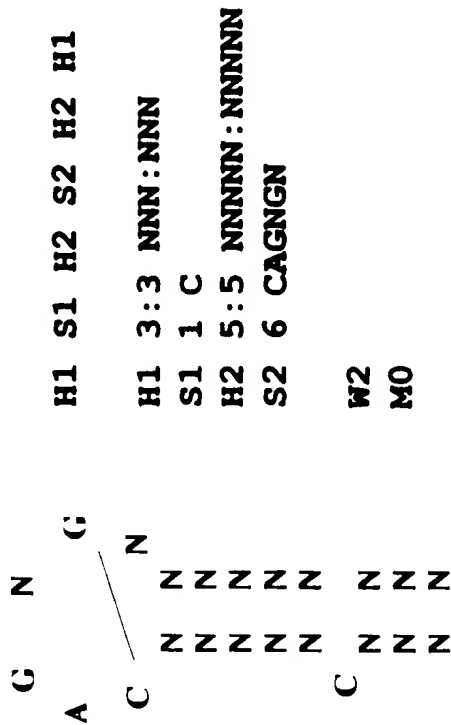
Figure 8

IRE String descriptor

This descriptor allows for

- a wobble (W) of 2
- no mismatches.
- N can be any nucleotide
- H refers to the stem region
- S refers to the single stranded region.

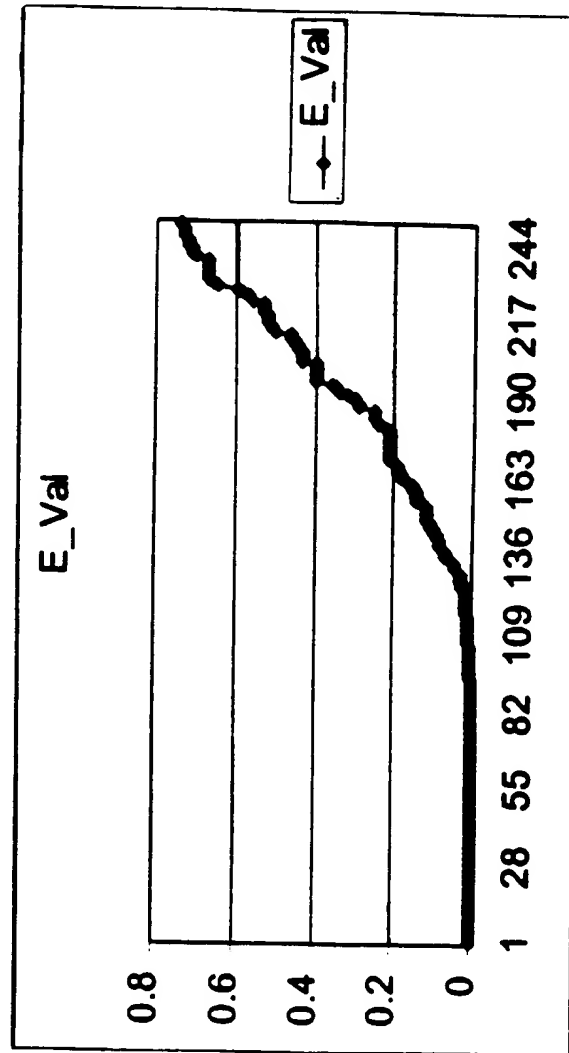
Figure 9



IRE Stem-loop Model

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Figure 10



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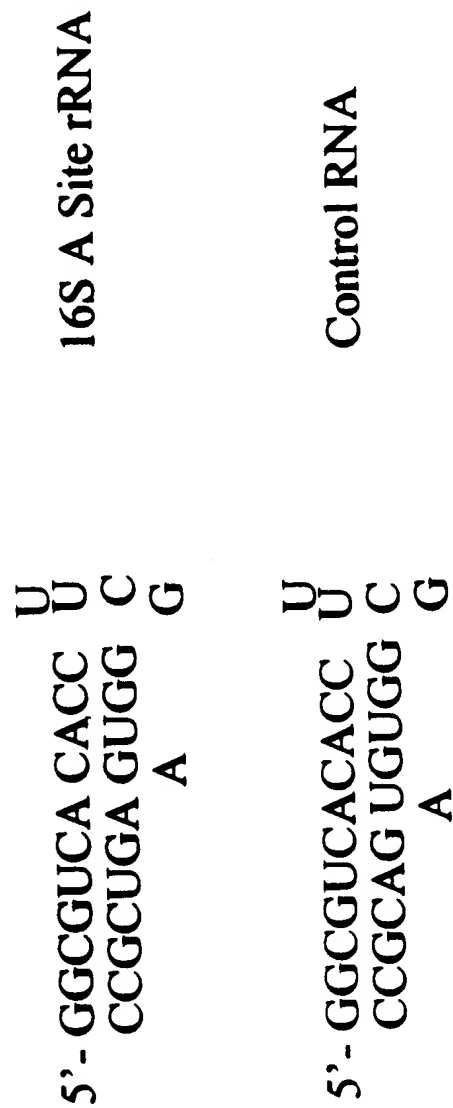


Figure 40

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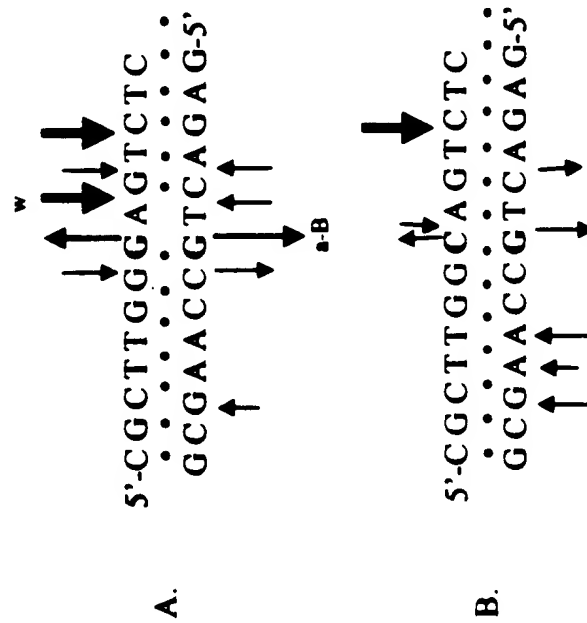


Figure 47

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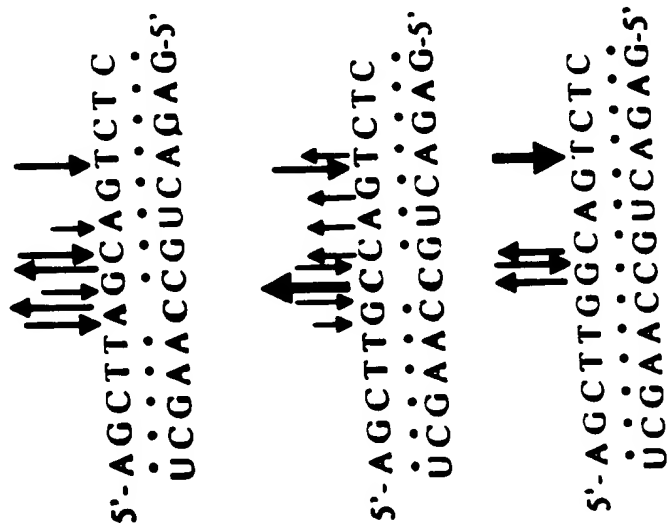


Figure 48 MS Fragmentation of DNA:RNA duplexes

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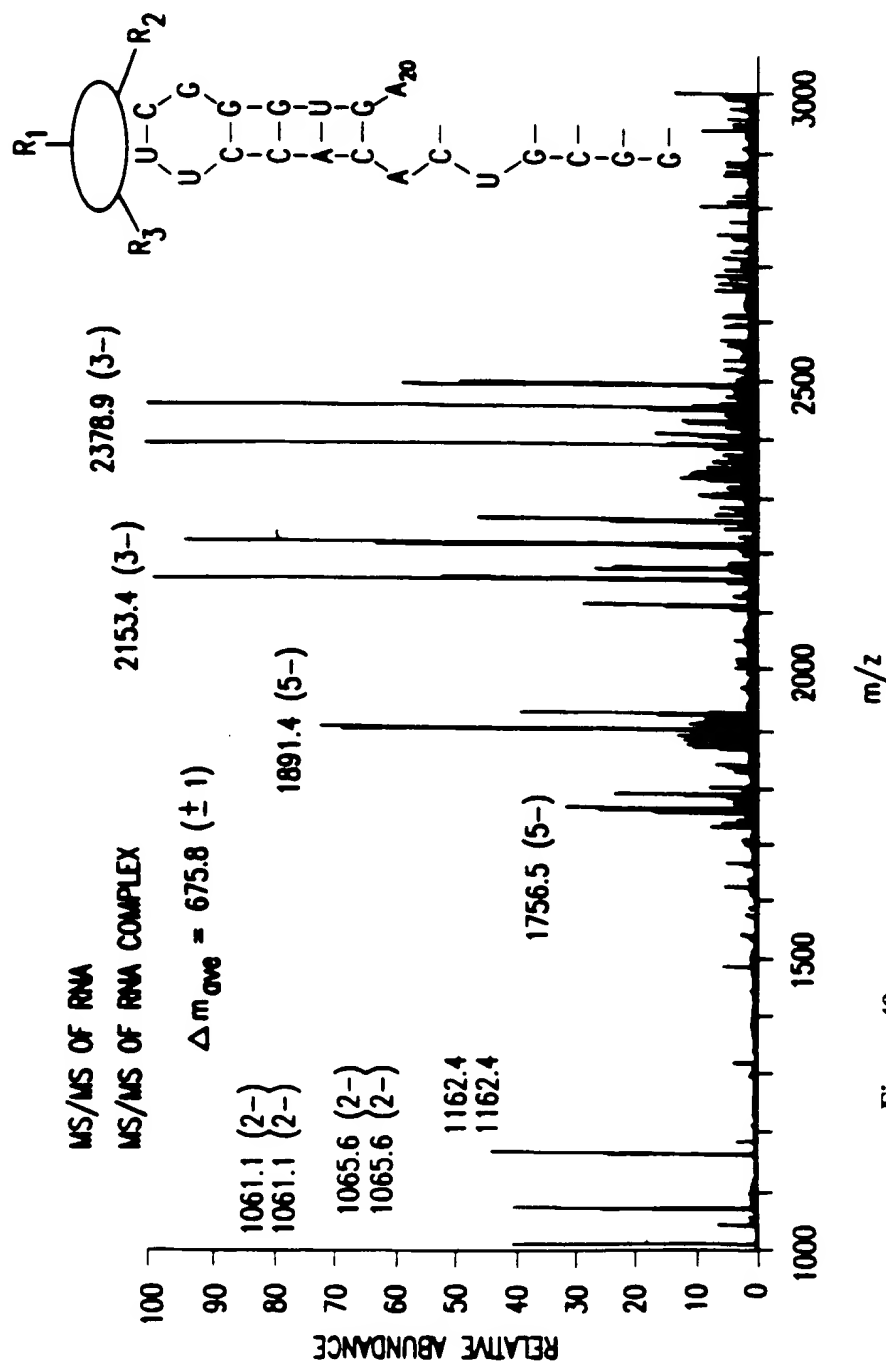


Figure 49

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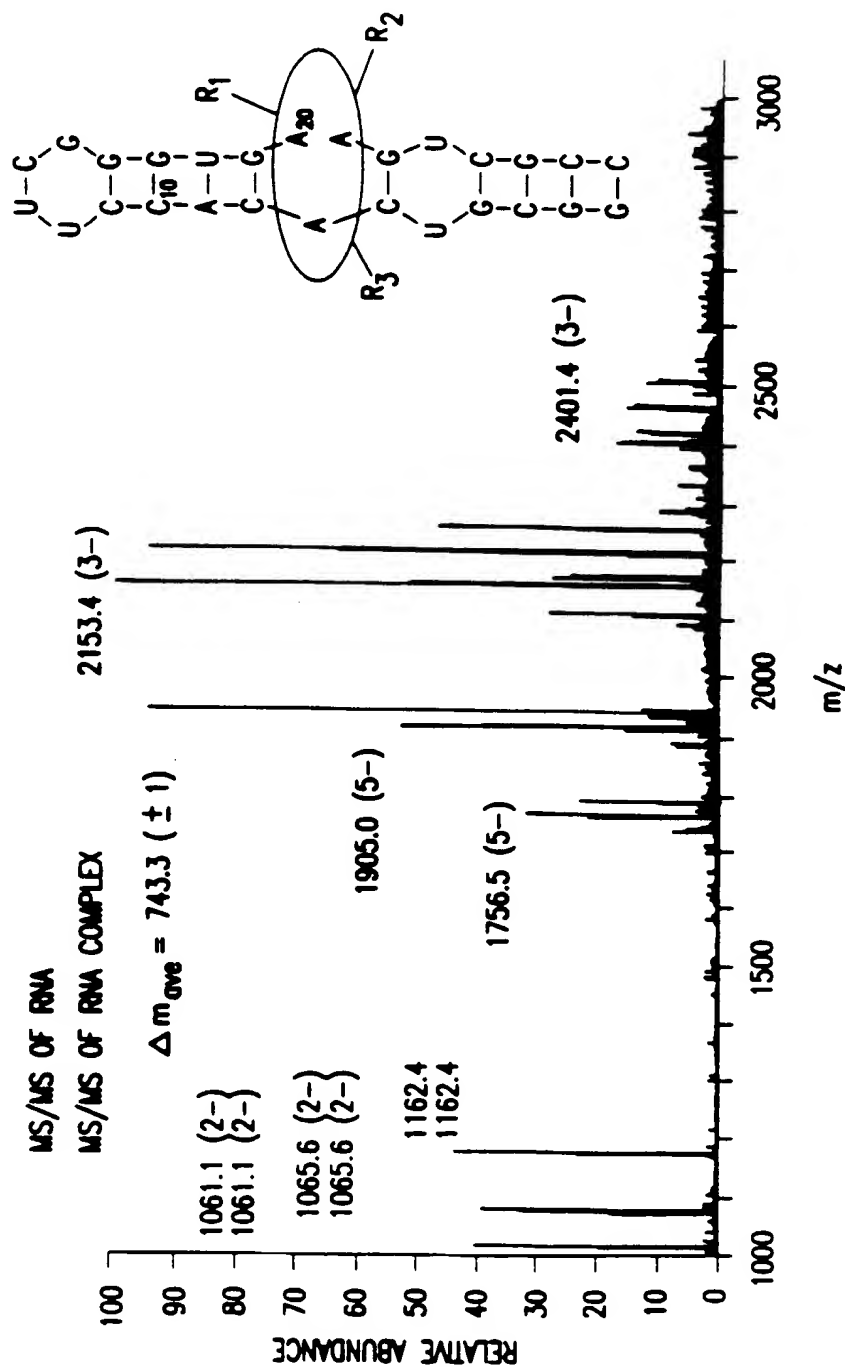


Figure 50

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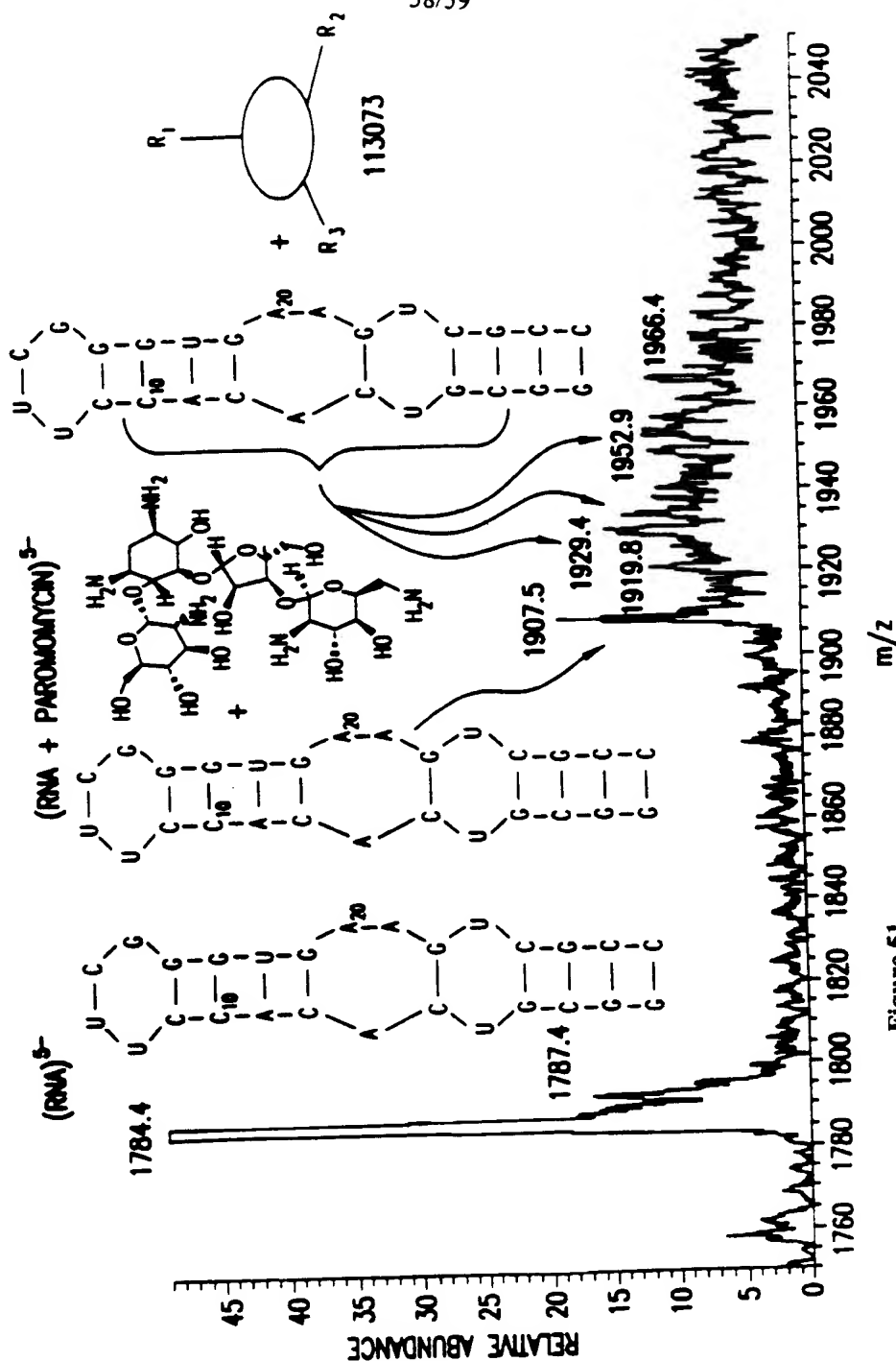


Figure 51

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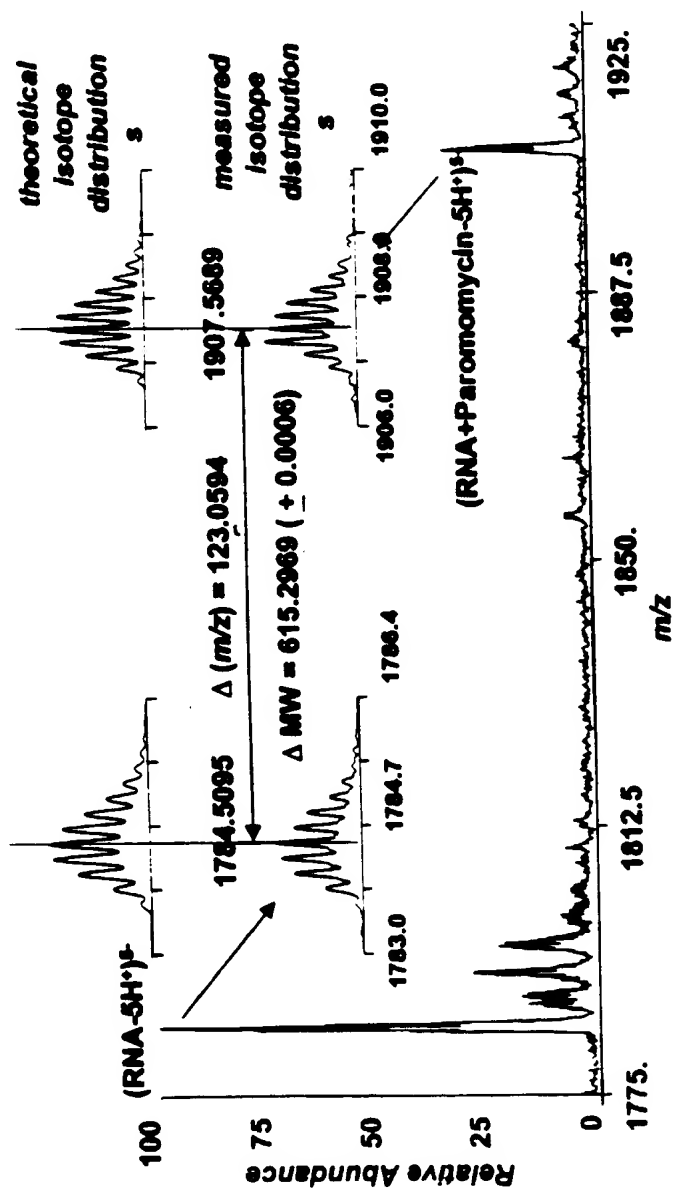


Figure 52

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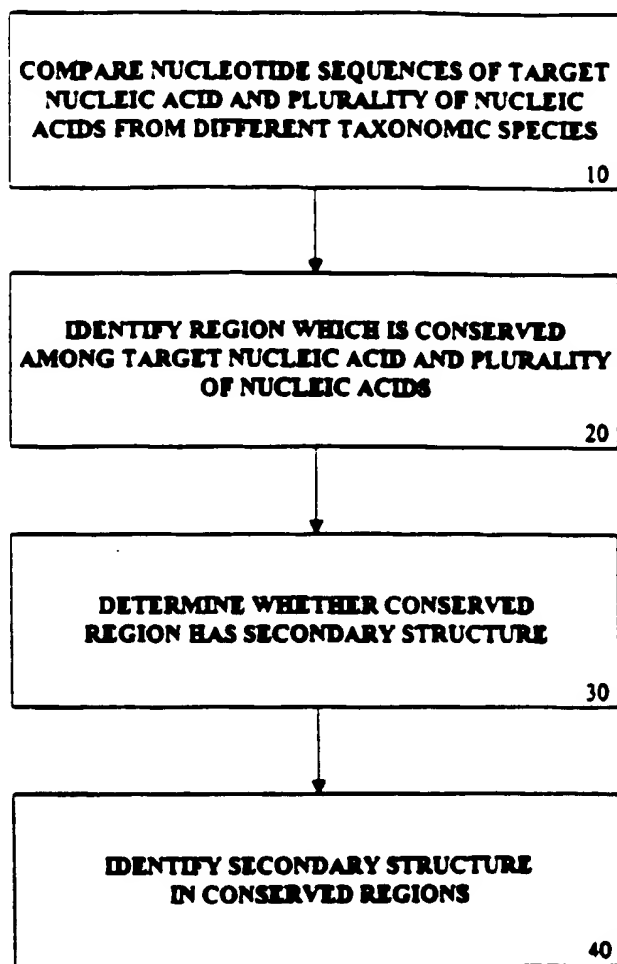


FIGURE 1

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Find Neighbors
and Assemble
Flow Diagram

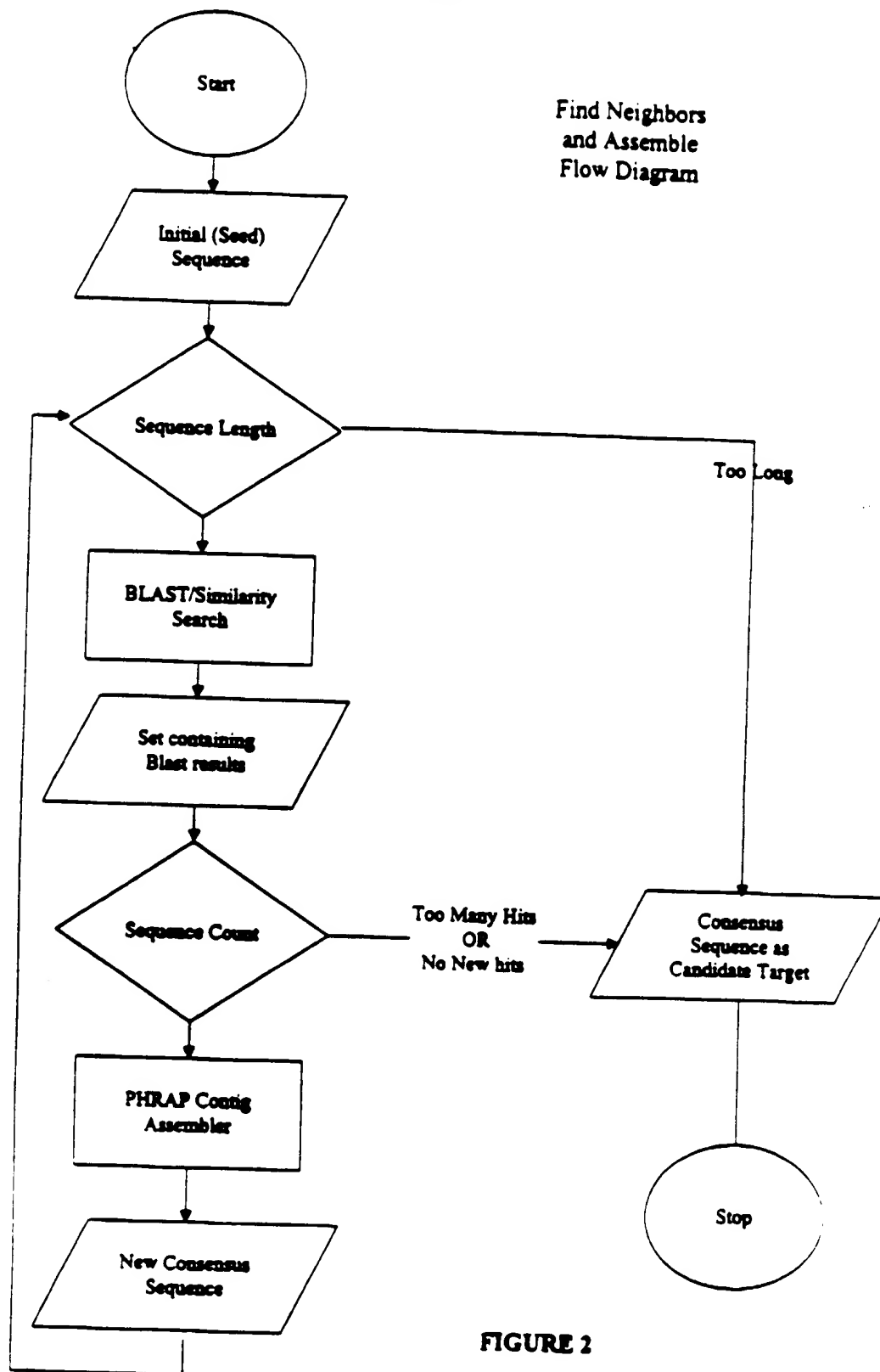


FIGURE 2

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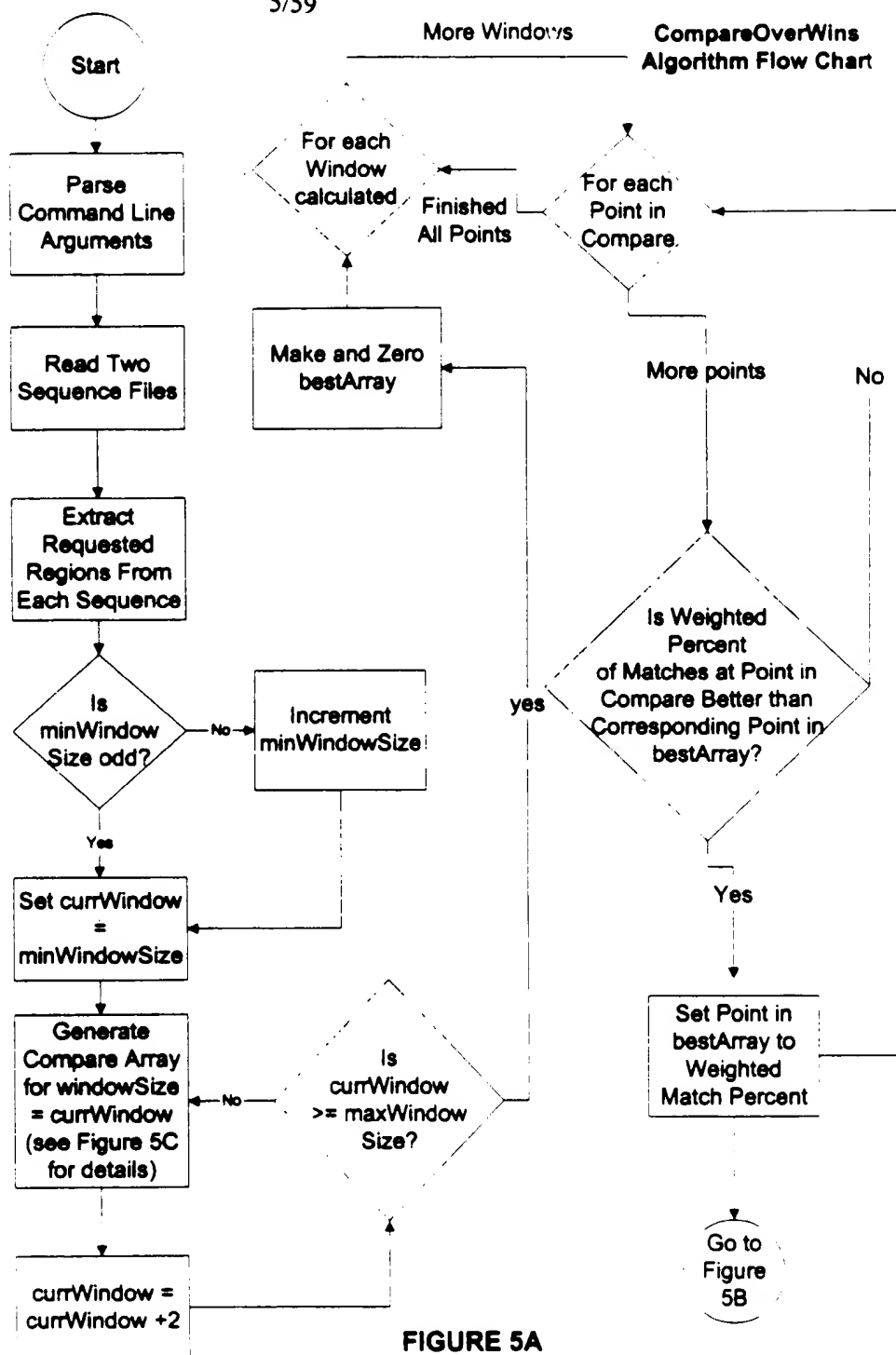
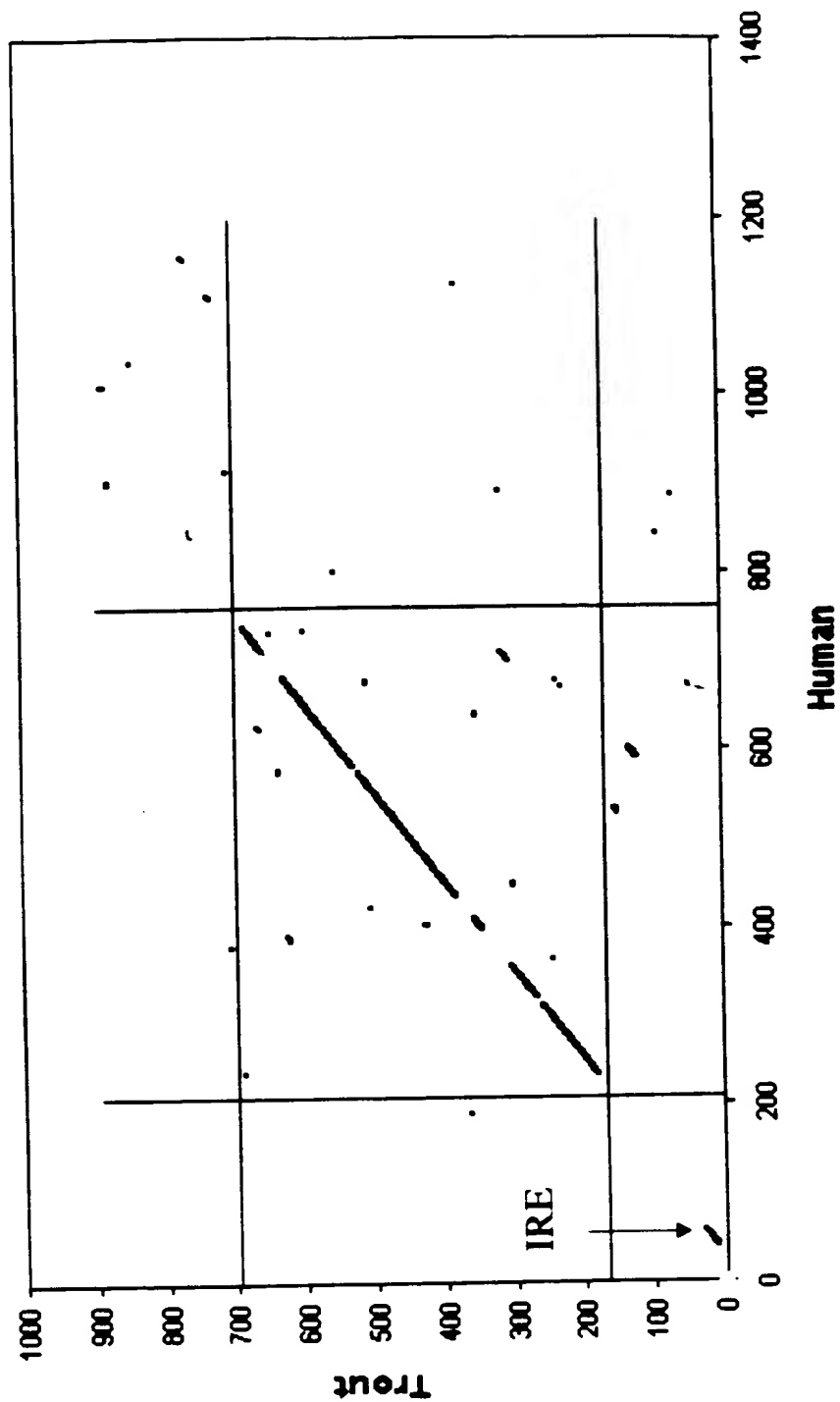


FIGURE 5A

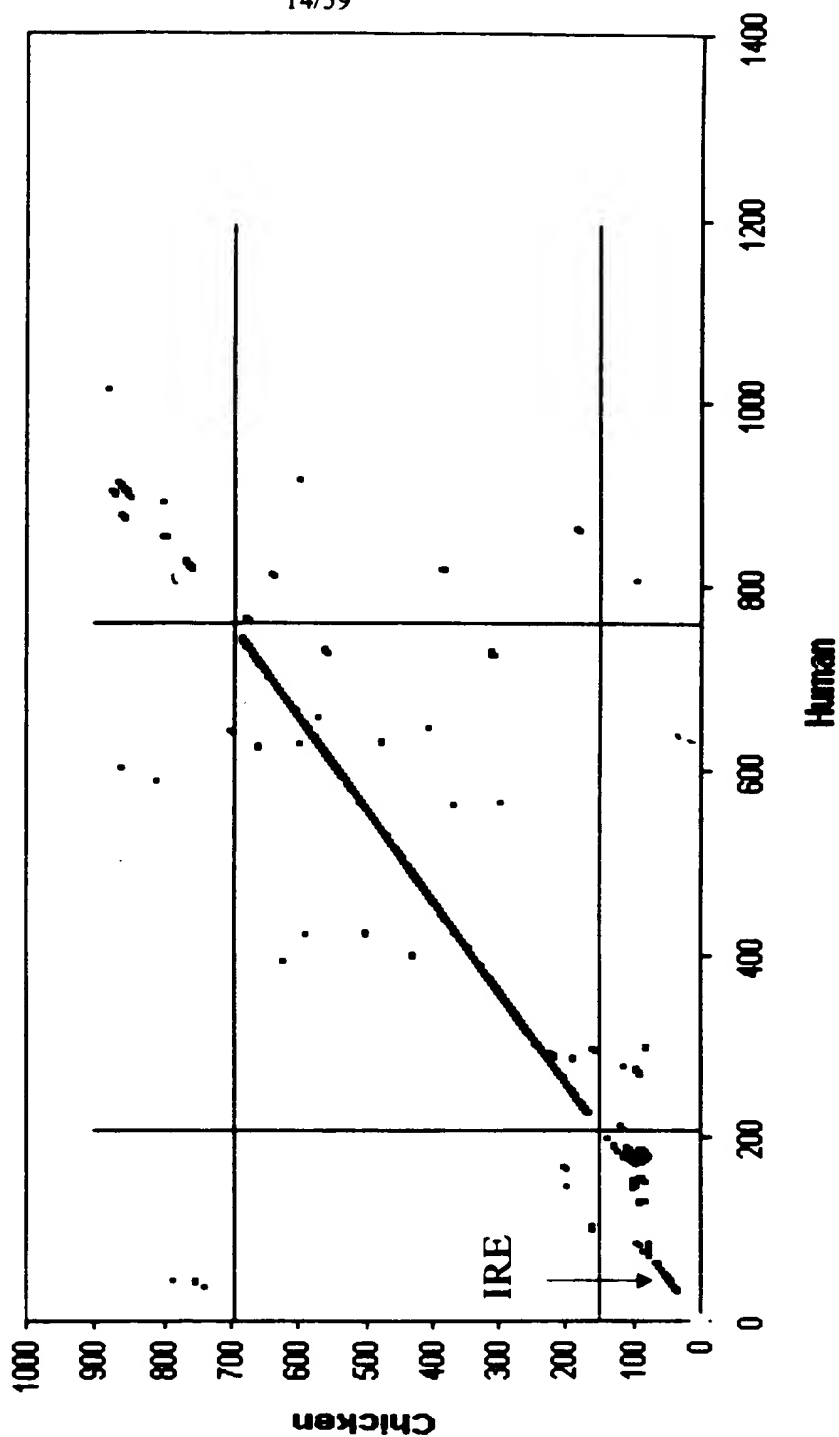
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Figure 11



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Figure 12



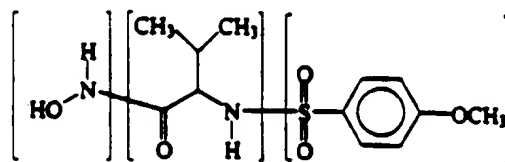
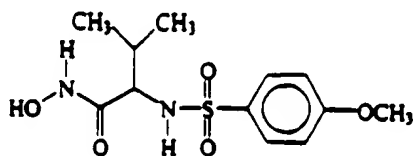
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	HUMAN PIC	HAMSTER MOUSE RAT	CHICKEN	TROUT SALMON	XENOPUS FROG	FLY	MOSQUITO
	G-U A C A U A U C G U G U A C	G-U A C A U A U C G U G U A C	G-U A C A U A U C G U G U A C	G-U A C A U A U C G U G U A C	G-U A C A U A U C G U G U A C	G-U A C A U A U C G U G U A C	G-U A C A U A U C G U G U A C
HUMAN PIC	No	No	Yes	Yes	Yes	No	No
HAMSTER MOUSE RAT		No	Yes	Yes	Yes	No	No
CHICKEN			No	Yes	Yes	No	No
TROUT SALMON				No	Yes	Yes	Yes
XENOPUS FROG					No	Yes	Yes
FLY						No	Yes
MOSQUITO							No

Figure 13

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Compound CI



	Fi	Fii	Fiii
Molecular formula	H_2NO	C_3H_7NO	$C_7H_7O_3S$

Figure 14

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Addition of fragments to yield compounds

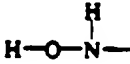
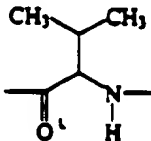
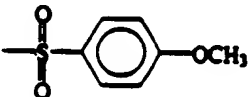
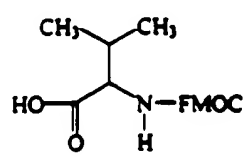
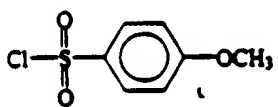
Fragment Identifier	Table			
	Structure	Name	Molecular formula	Other
F _i		Hydroxylamine	H ₂ NO	...
F _{ii}		Amino acid	C ₅ H ₉ NO	...
F _{iii}		Sulfonyl	C ₇ H ₇ O ₂ S	...

Figure 15

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Reagents	Identifier	Name	Properties
$\text{H}-\text{O}-\text{NH}_2$ or $\textcircled{\text{P}}-\text{O}-\text{NH}_2$	R_i	Hydroxylamine	...
	R_{ii}	FMOC blocked amino acid	...
	R_{iii}	Sulfonylchloride	...

$\textcircled{\text{P}}$ = Solid support

Figure 16

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Transformation

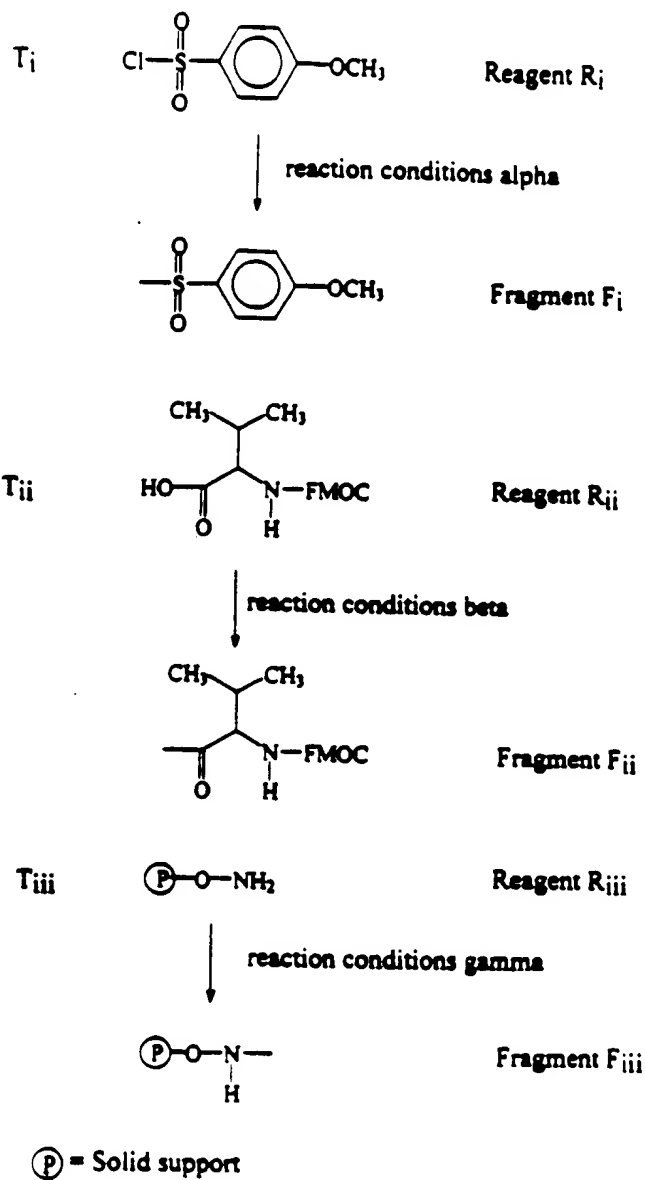


Figure 17

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Common Fragment / Different Reagents and Transformations

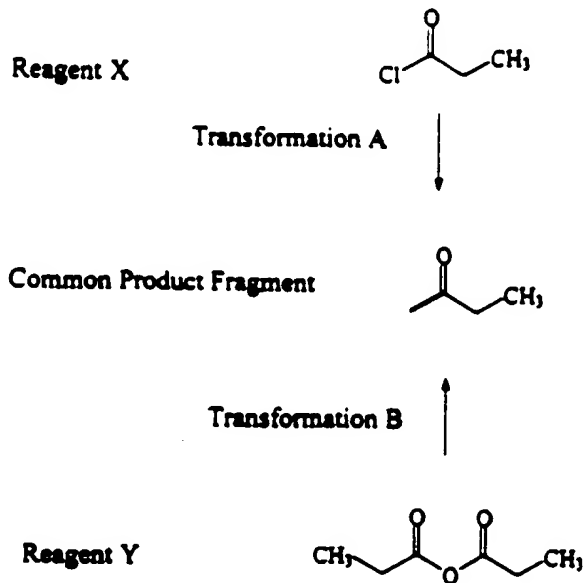


Figure 18

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Common Fragment / Different Reagents and Transformations

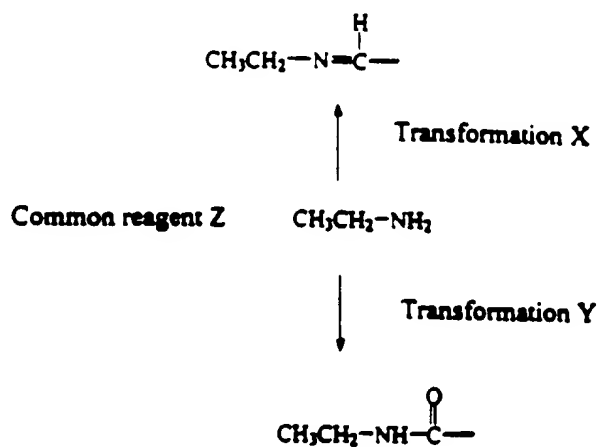


Figure 19A

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Common Reagent

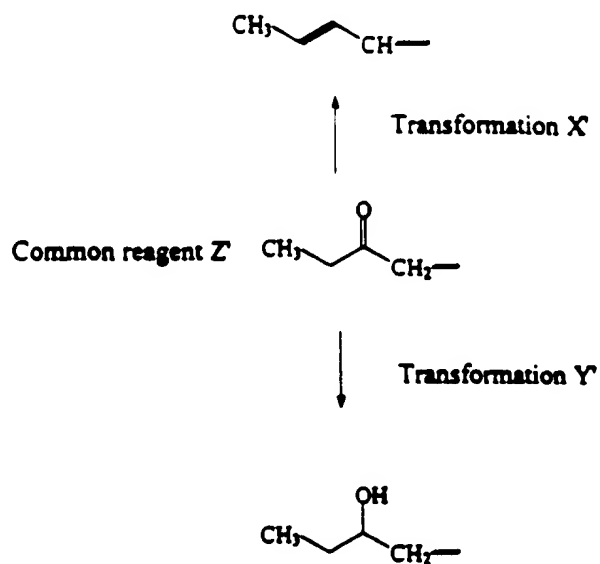


Figure 19B

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Symbolic addition of fragments to yield compound



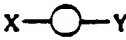
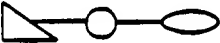
<u>Symbolic Structure</u>	<u>Symbolic Identifier</u>	<u>Molecular formula</u>
Fragment		
	F_i'	$C_uH_vN_w \dots$
	F_{ii}'	$C_uH_vN_w \dots$
	F_{iii}'	$C_uH_vN_w \dots$
Compound		
	CT'	$C_uH_vN_w \dots$
		$ \begin{aligned} &\text{Molecular formula } F_i' \\ &\quad + \\ &\text{Molecular formula } F_{ii}' \\ &\quad + \\ &\text{Molecular formula } F_{iii}' \\ &\hline &= \text{Molecular formula } CT' \end{aligned} $

Figure 20

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Symbolic Reagent Table


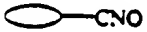


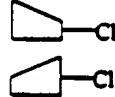
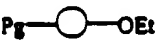


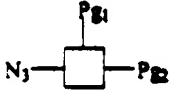
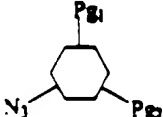
<u>Identifier</u>	<u>Name</u>	<u>Structure</u>	<u>Molecular formula</u>
R1	xxx		xxx
R2	...		...
R3	...		...
R4	...		...
R5	...		...
R6	...		...
R7	...		...
R8	...		...
R9	...		...
R10	...		...

Figure 21

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Symbolic Fragment Table




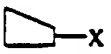
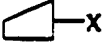
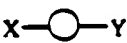

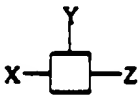
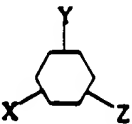
Identifier	Symbolic Structure	Molecular formula	Molecular Weight
F1		xxx	xxx
F2	
F3	
F4	 
F5	
F6	
F7	
F8	

Figure 22

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Symbolic Transformation Table



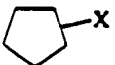

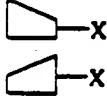




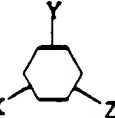
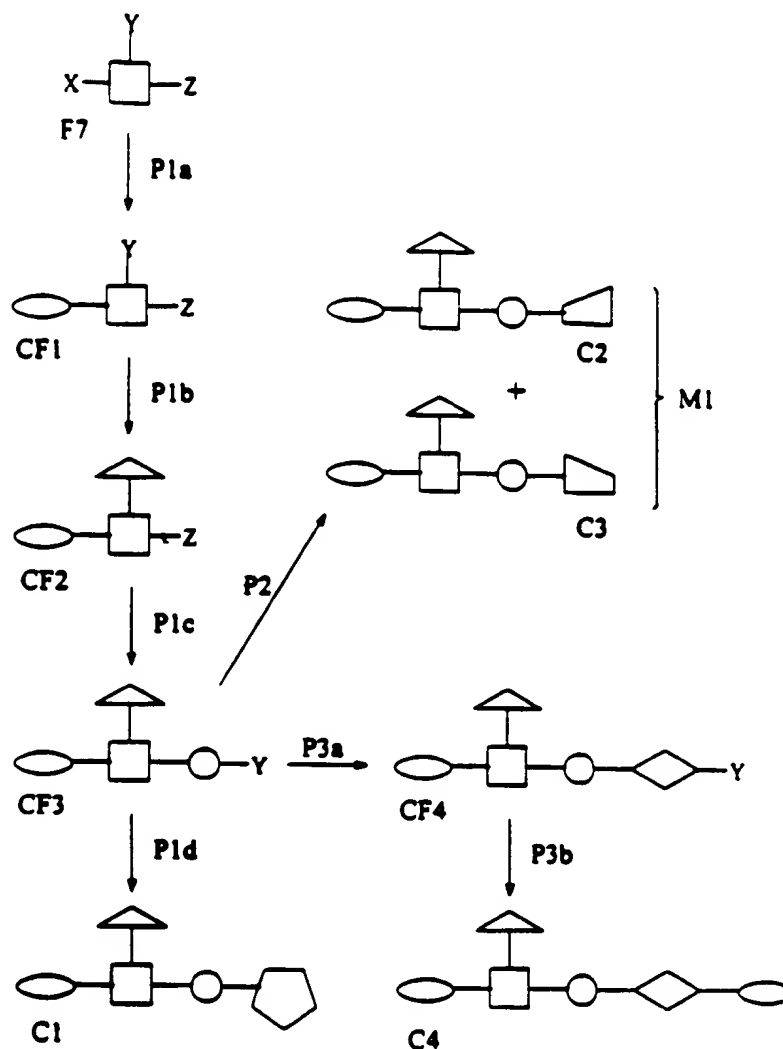
<u>Identifier</u>		<u>Symbolic Reactions</u>	<u>Reagent</u>
T1	F1	 X \leftarrow R1	conditions α
T2	F2	 X \leftarrow R2	conditions β
T3	F3	 X \leftarrow R3	conditions α
T4	F3	 X \leftarrow R4	conditions α
T5	F4	 X \leftarrow R5	conditions α
T6	F5	X —  — Y \leftarrow R6	conditions ϵ
T7	F5	X —  — Y \leftarrow R7	conditions α
T8	F6	X —  — Y \leftarrow R8	conditions α
T9	F7	X —  — Z \leftarrow R9	conditions γ
T10	F8	X —  — Z \leftarrow R10	conditions γ

Figure 23

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Single Compounds and Mixtures



P = synthetic path CF = complex fragment
 F = fragment M = mixture
 C = compound

Figure 24

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Mixture 2

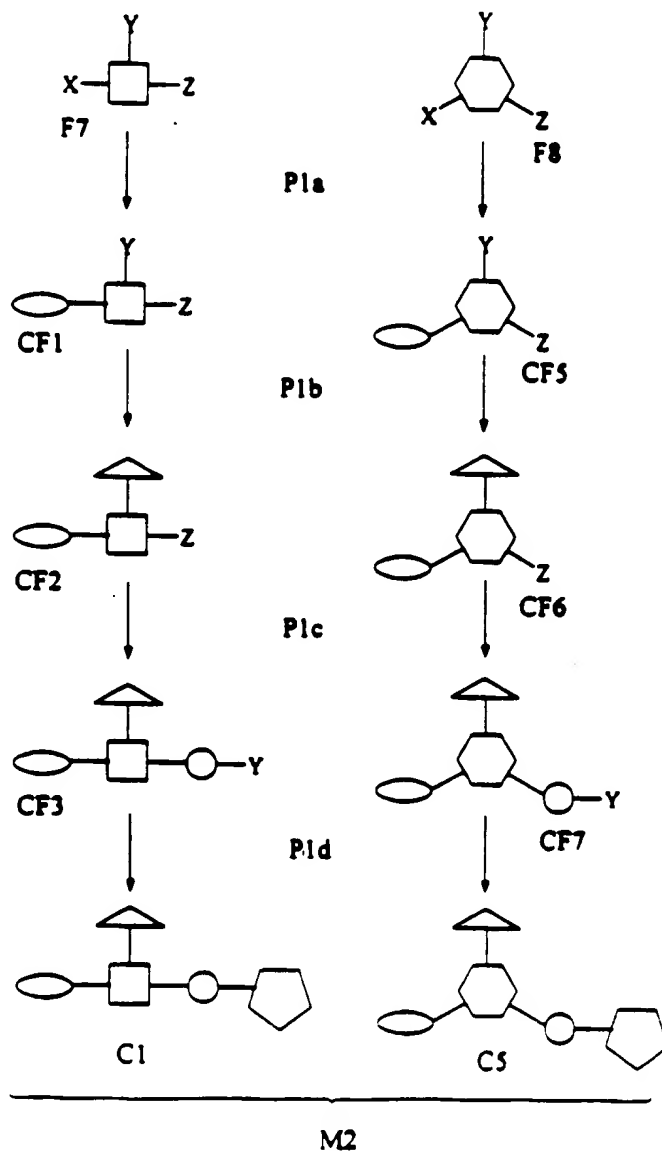


Figure 25

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Mixture 3

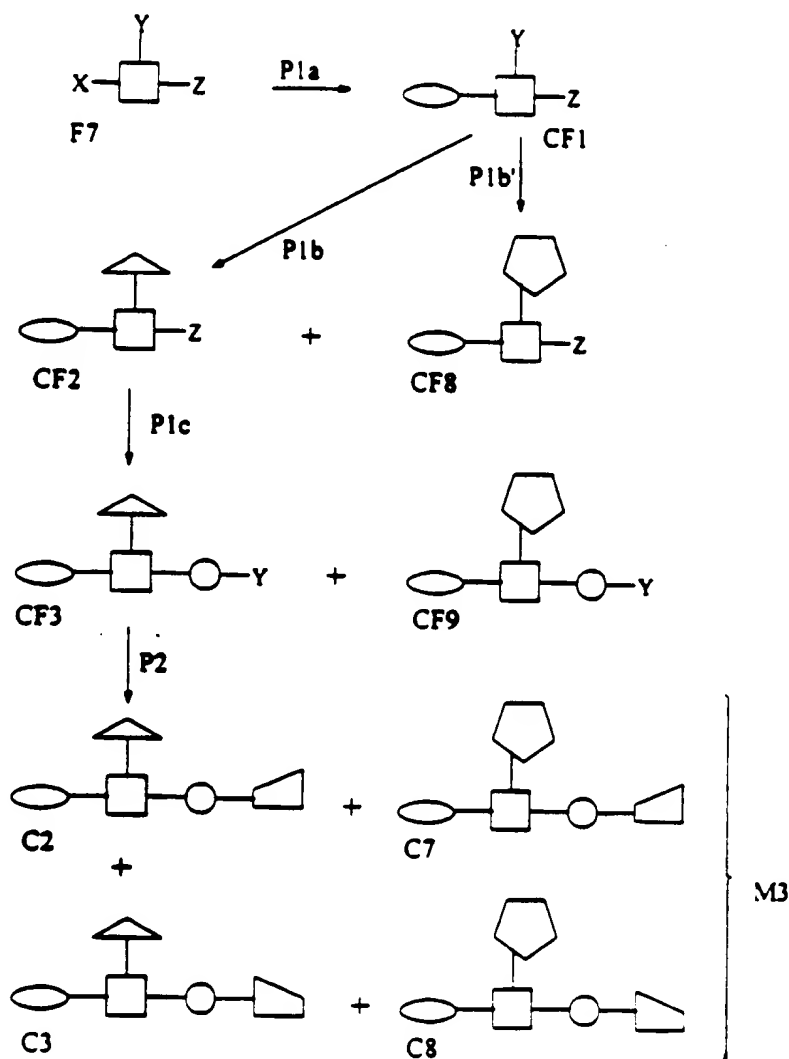
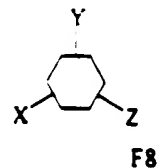
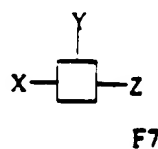


Figure 26

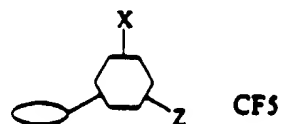
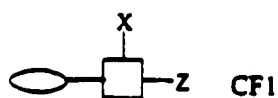
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Mixture 4

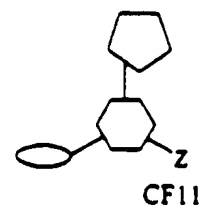
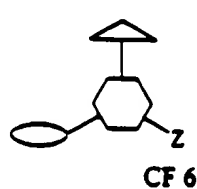
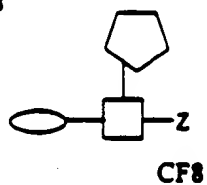
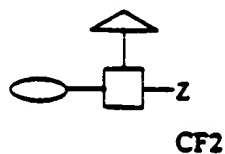
2 Starting Fragments



2 Complex Fragments



4 Complex Fragments



8 Complex Fragments

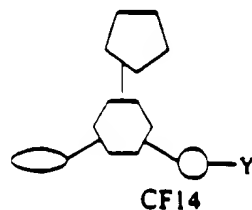
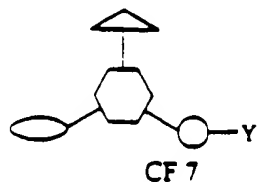
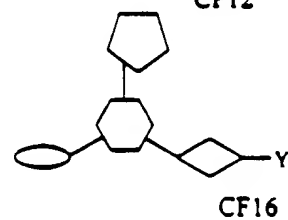
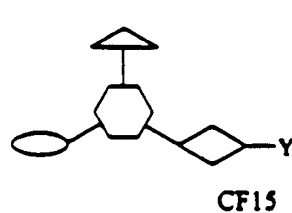
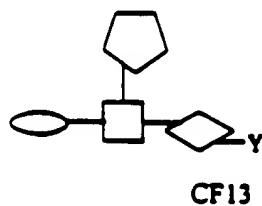
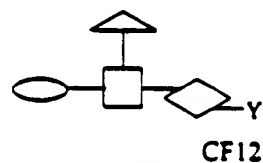
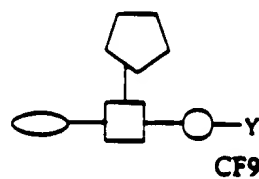
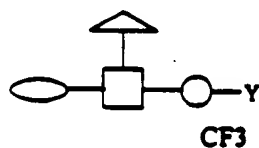


Figure 27A

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Mixture 4 (continued)

16 compounds

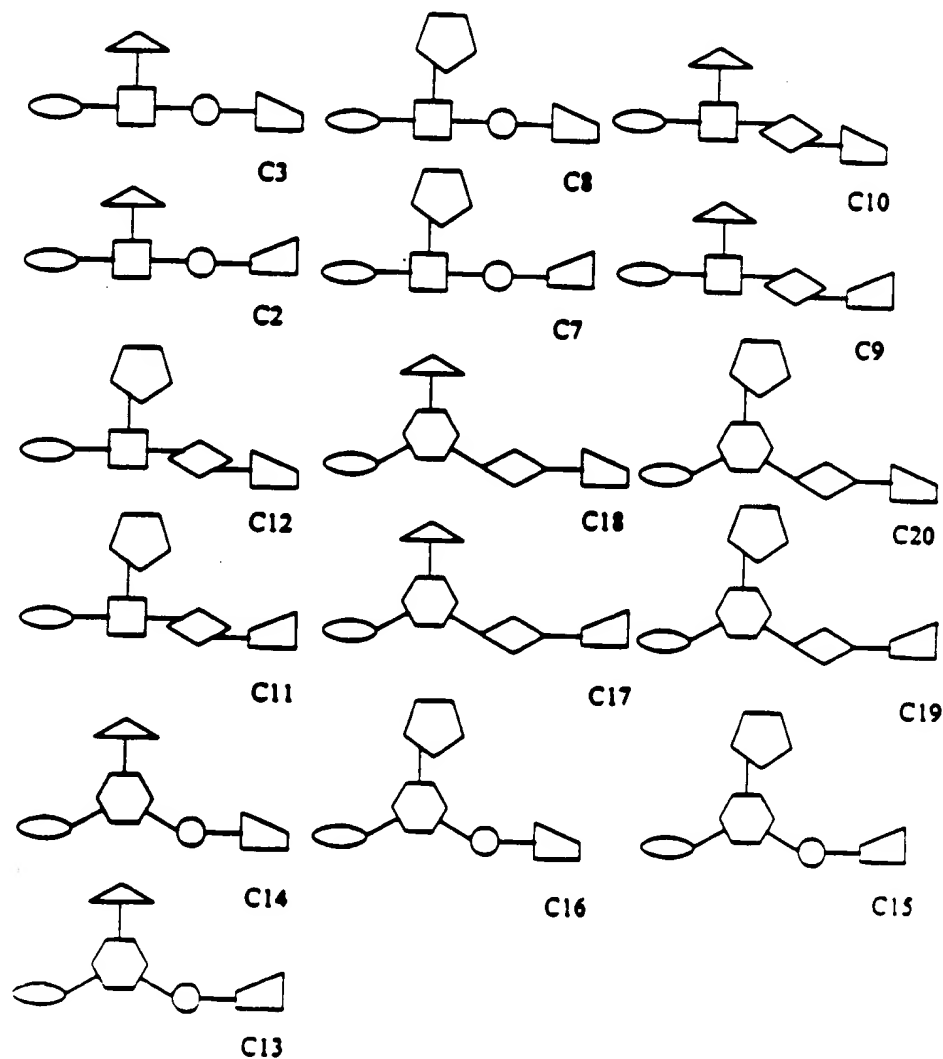


Figure 27B

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Tracking Table for Compound C1

(a) By Fragments:

n	n+1	n+2
F7	F2 F1 F5	F3

(b) By Transformations:

Synthesis Path 1

n	n+1	n+2
T9	T2 T1 T6	T3

Synthesis Path 2

n	n+1	n+2
T9	T2 T1 T7	T3

Synthesis Path 3

n	n+1	n+2
T9	T2 T1 T6	T4

Synthesis Path 4

n	n+1	n+2
T9	T2 T1 T7	T4

Figure 28

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Tracking Table

Tracking M1

Step 1		
T9		
Step 2		
T9	T2	
Step 3		
T9	T2 T1	
Step 4		
T9	T2 T1 T7	
Step 5		
T9	T2 T1 T7	TS ¹
C2		
Step 5		
T9	T2 T1 T7	TS ²
C3		

Figure 29

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Tracking Table

Tracking M2

Step 1			Step 1		
n	n+1	n+2	n	n+1	n+2
T9			T10		
Step 2			Step 2		
n	n+1	n+2	n	n+1	n+2
T9	T2		T10	T2	
Step 3			Step 3		
n	n+1	n+2	n	n+1	n+2
T9	T2 T1		T10	T2 T1	
Step 4			Step 4		
n	n+1	n+2	n	n+1	n+2
T9	T2 T1 T7		T10	T2 T1 T7	
Step 5			Step 5		
n	n+1	n+2	n	n+1	n+2
T9	T2 T1 T7	T4	T10	T2 T1 T7	T4
C1			C5		

Figure 30

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Tracking Table

Tracking M3

Step 1

T9		
----	--	--

Step 2

T9	T2	
----	----	--

Step 3

T9	T2 T1	
----	----------	--

Step 3

T9	T2 T3	
----	----------	--

Step 4

T9	T2 T1 T7	
----	----------------	--

Step 4

T9	T2 T3 T7	
----	----------------	--

Step 5

T9	T2 T1 T7	T5 ¹
----	----------------	-----------------

C2

Step 5

T9	T2 T1 T7	T5 ²
----	----------------	-----------------

C3

Step 5

T9	T2 T3 T7	T5 ¹
----	----------------	-----------------

C7

Step 5

T9	T2 T3 T7	T5 ²
----	----------------	-----------------

C8

Figure 31

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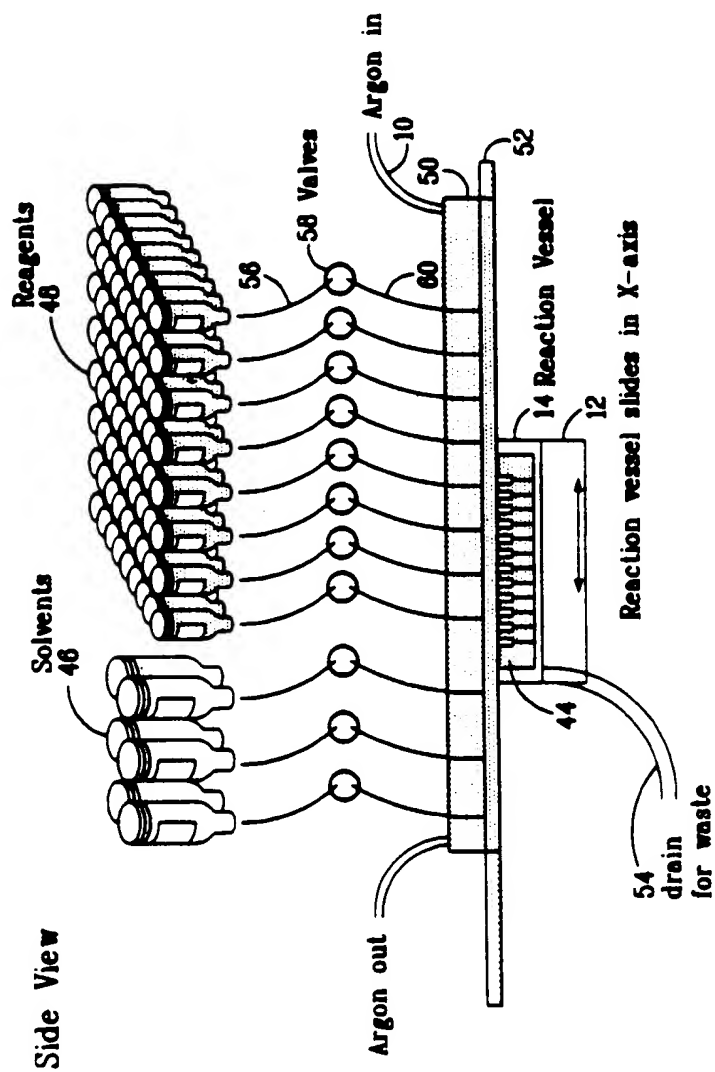


Figure 32

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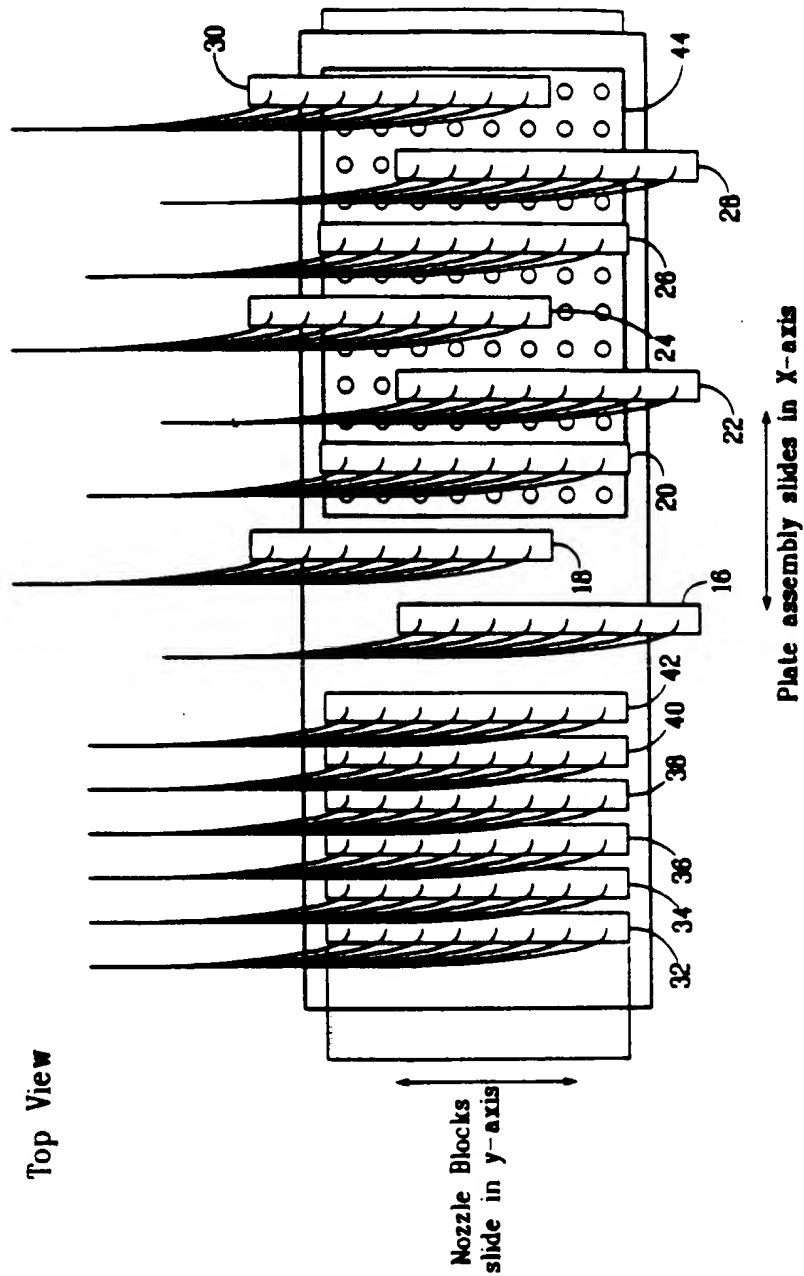


Figure 33

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Synthesis of hydroxamic acids from alcohol resin

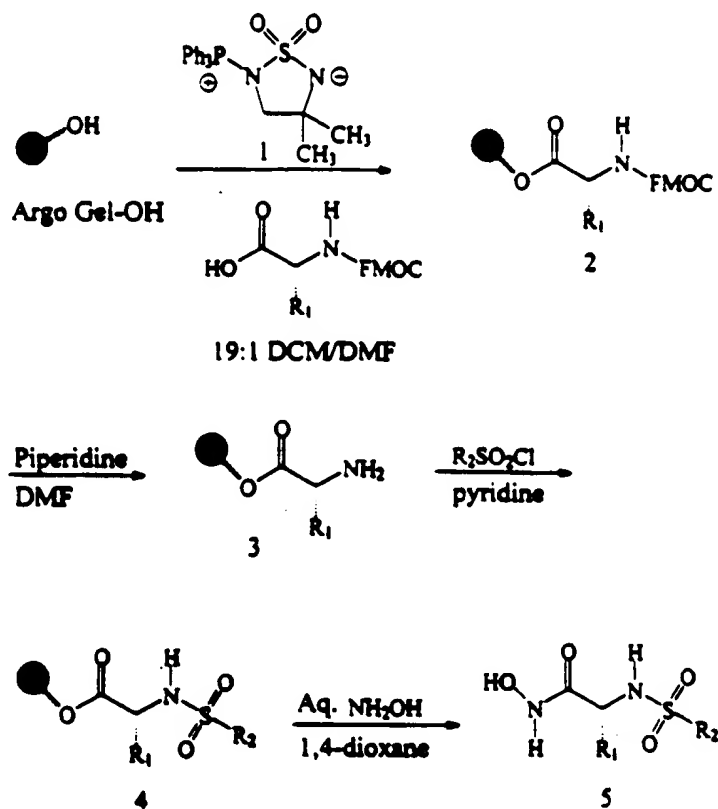


Figure 34

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Synthesis of hydroxamic acids from hydroxylamine resin

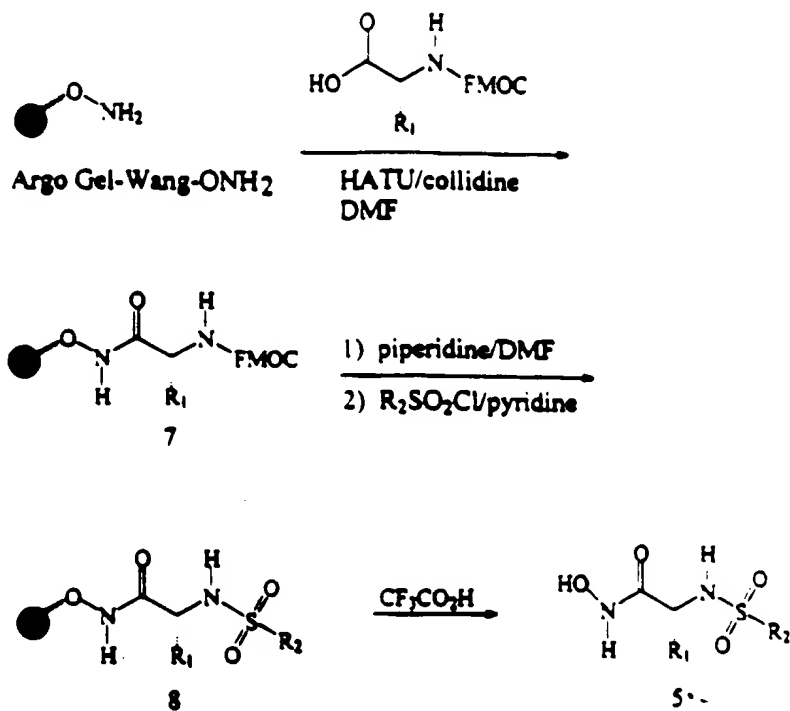


Figure 35

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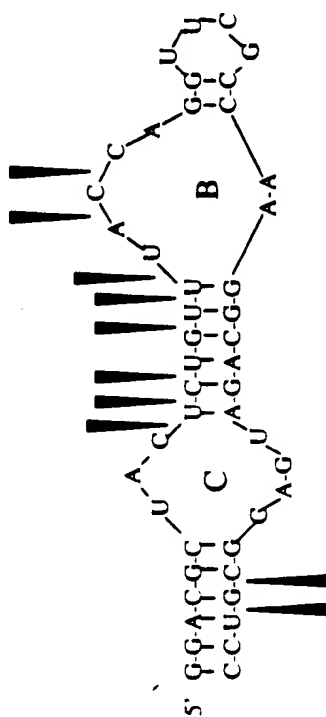


Figure 36

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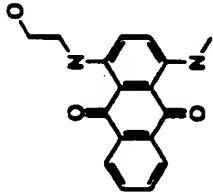
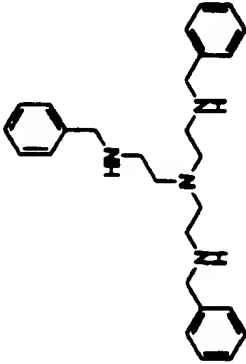
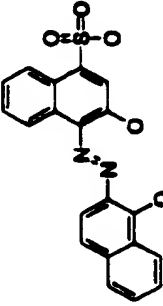
ACD Code	Structure	Calc. ΔG of binding (kcal/mole)	IC_{50} (μM)
00001199		-5.1	< 2
00192509		-8.5	< 2
00003934		-5.1	< 50

Figure 37

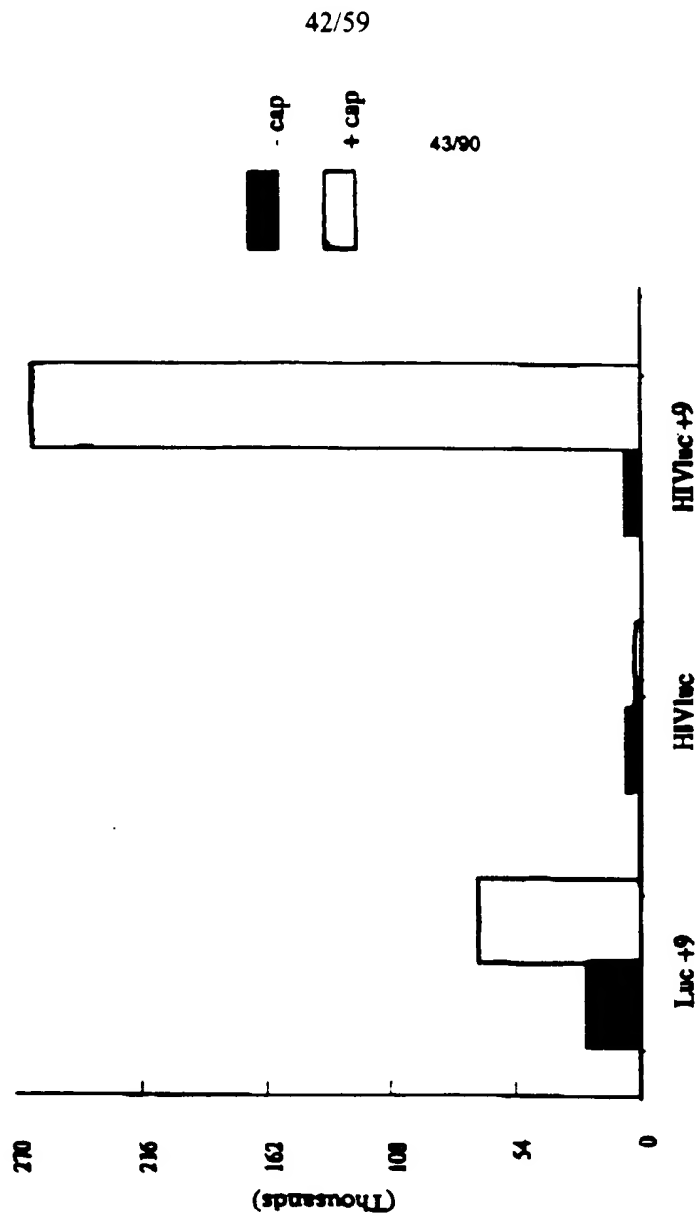


Figure 38A

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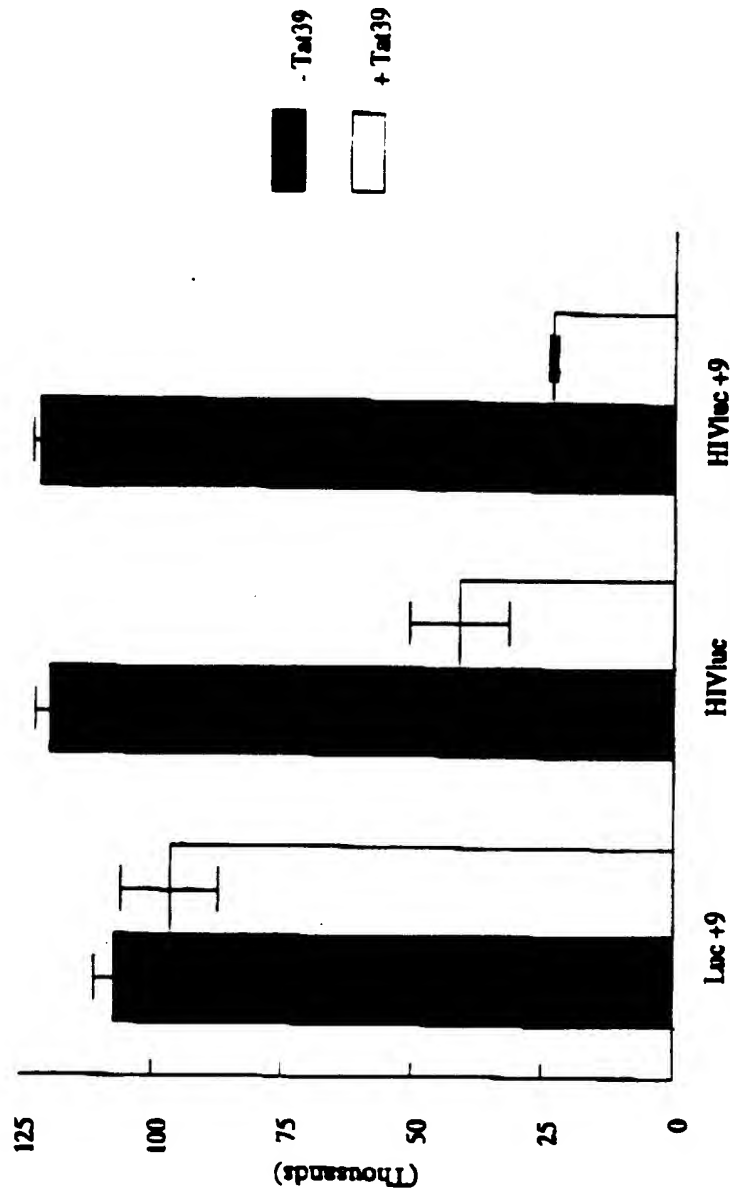
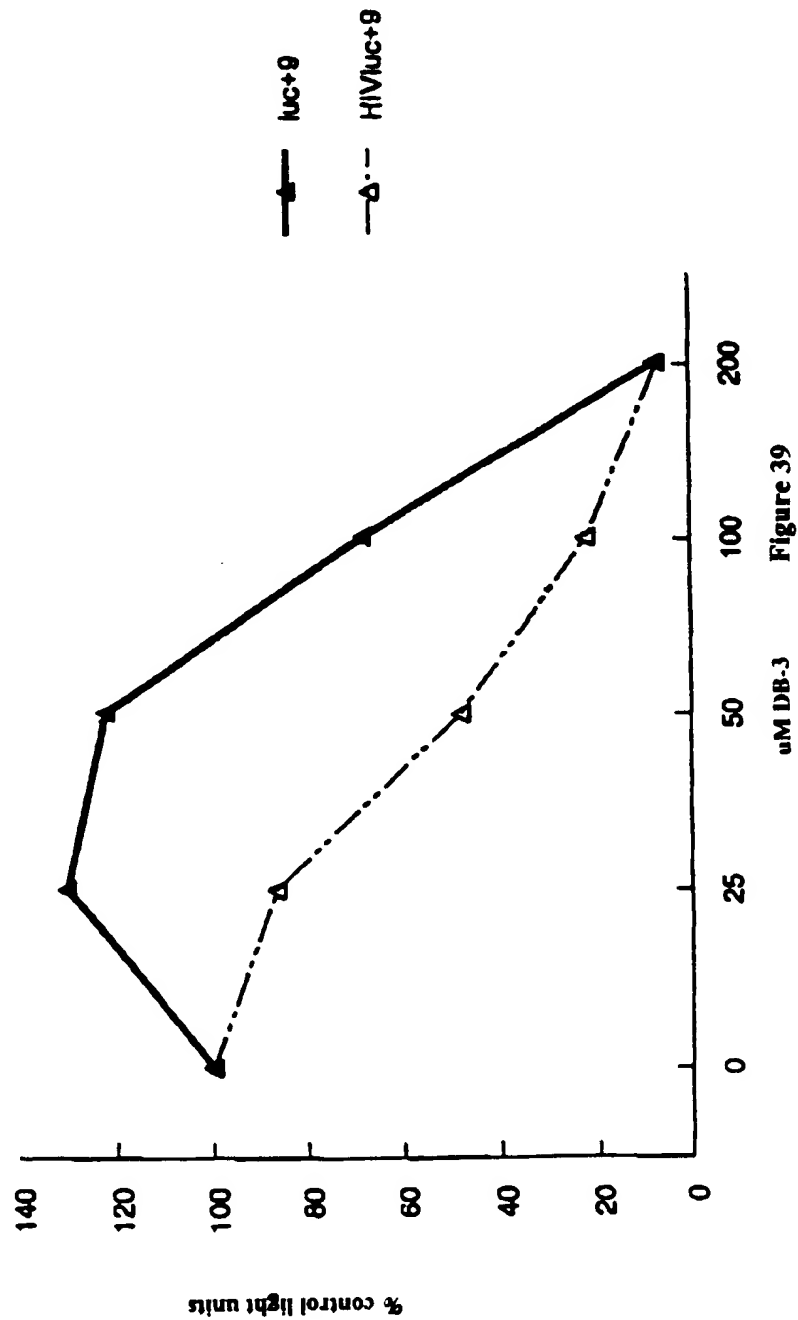


Figure 38B

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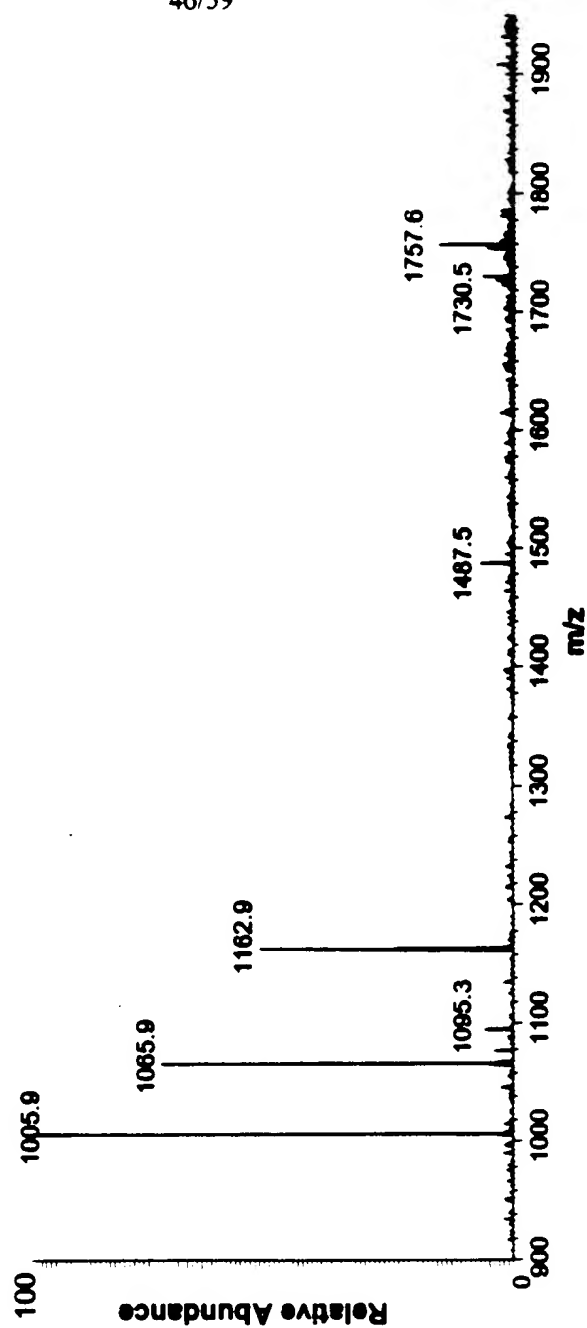


Figure 41A

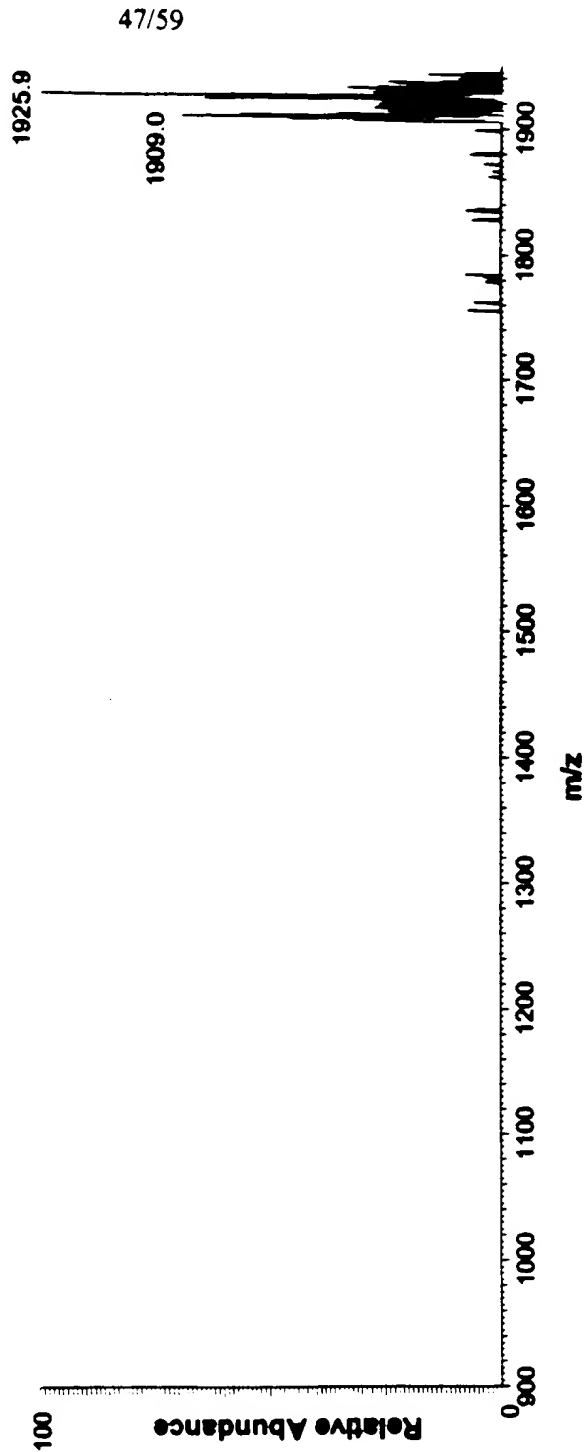


Figure 41B

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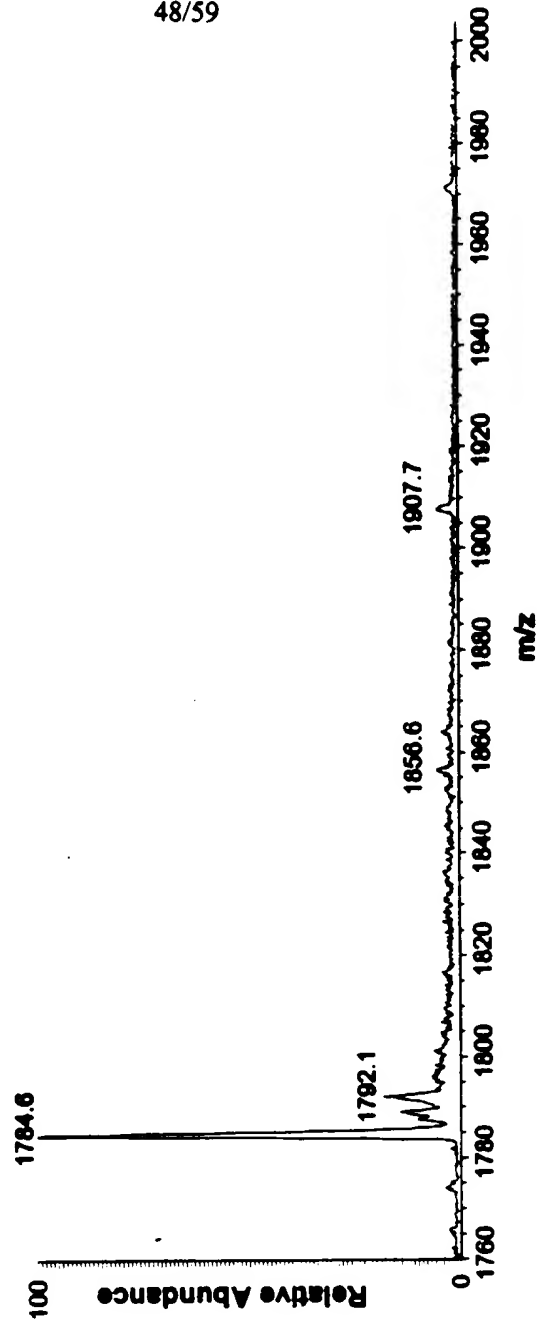


Figure 42A

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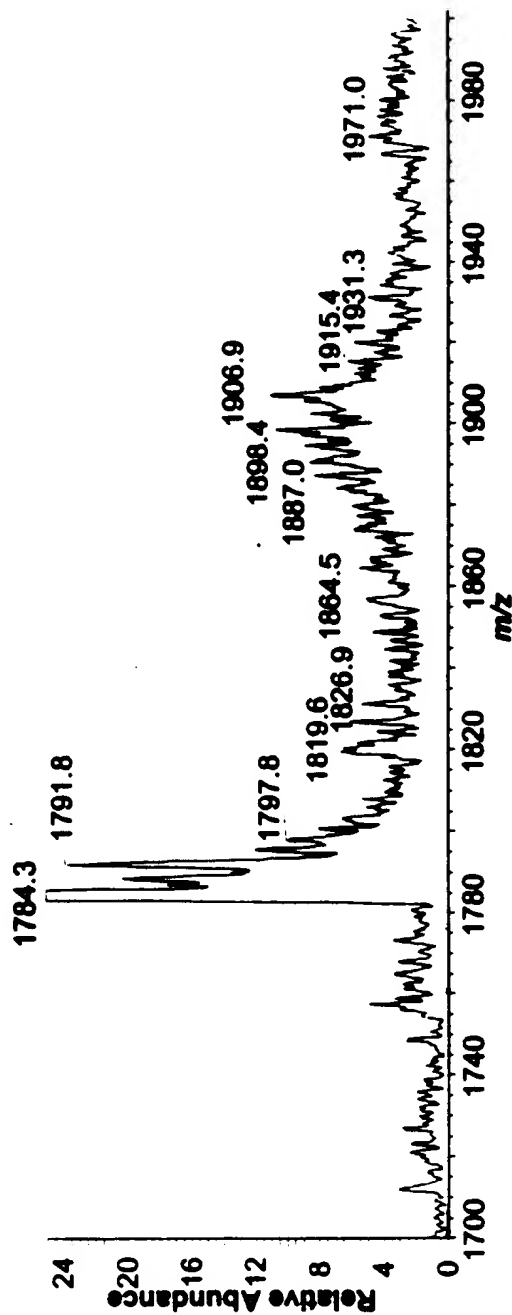


Figure 42B

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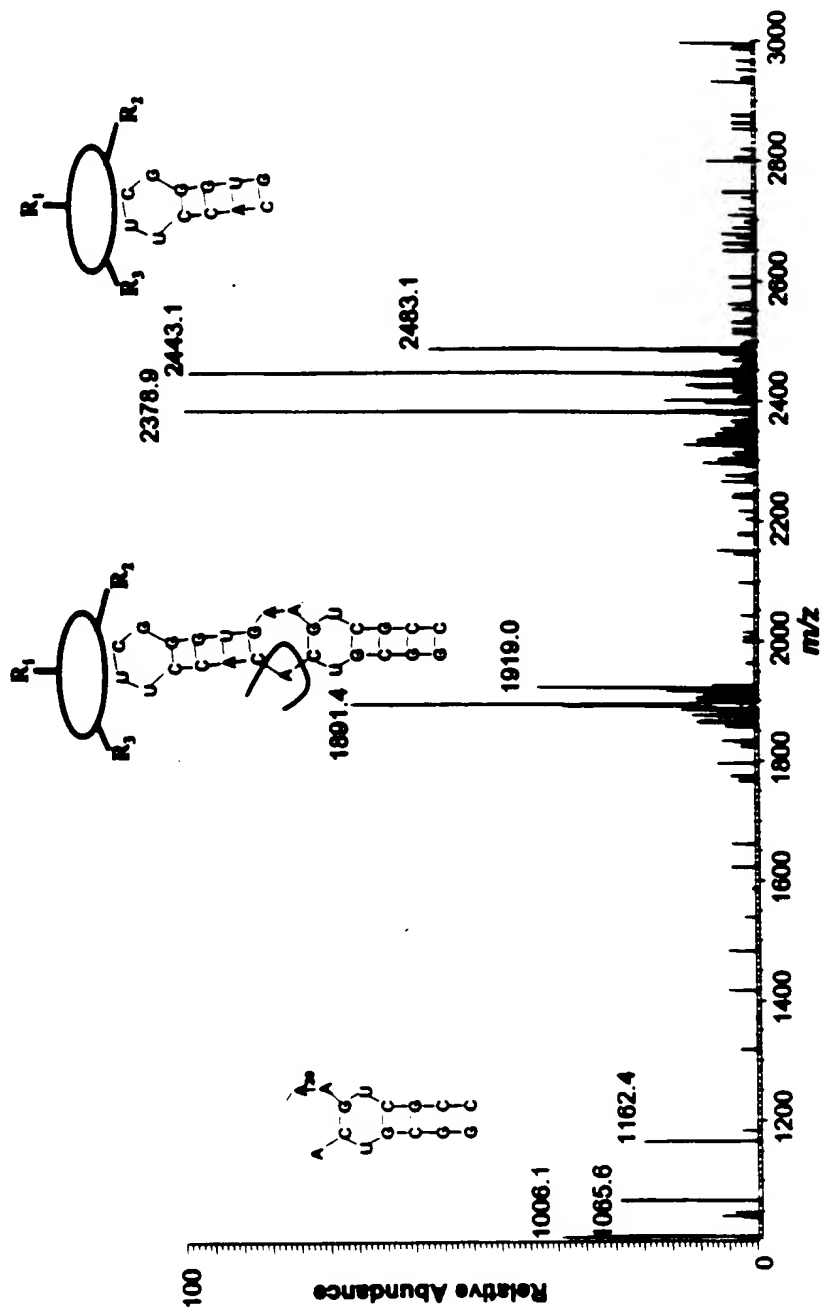


Figure 43

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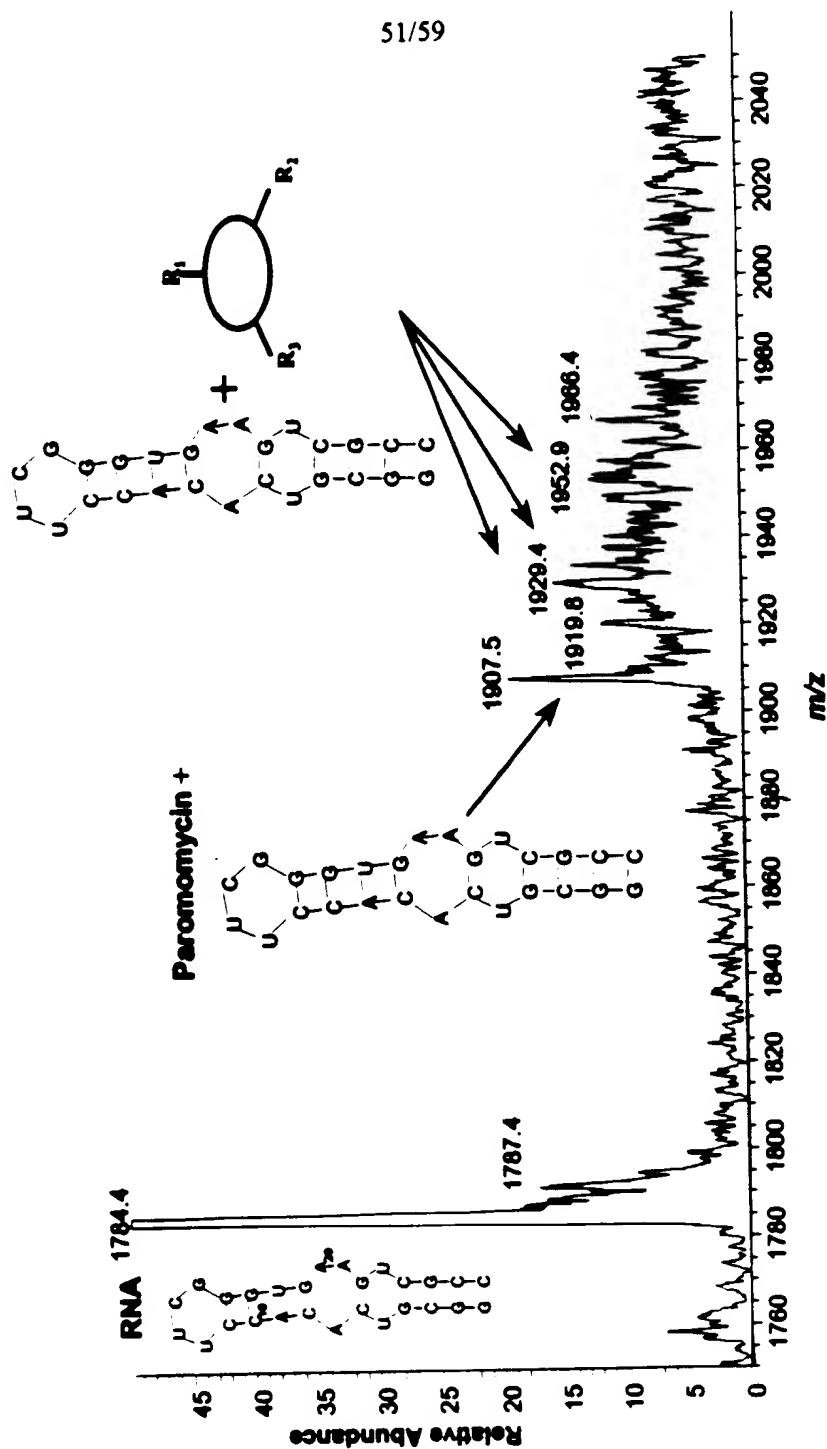


Figure 44

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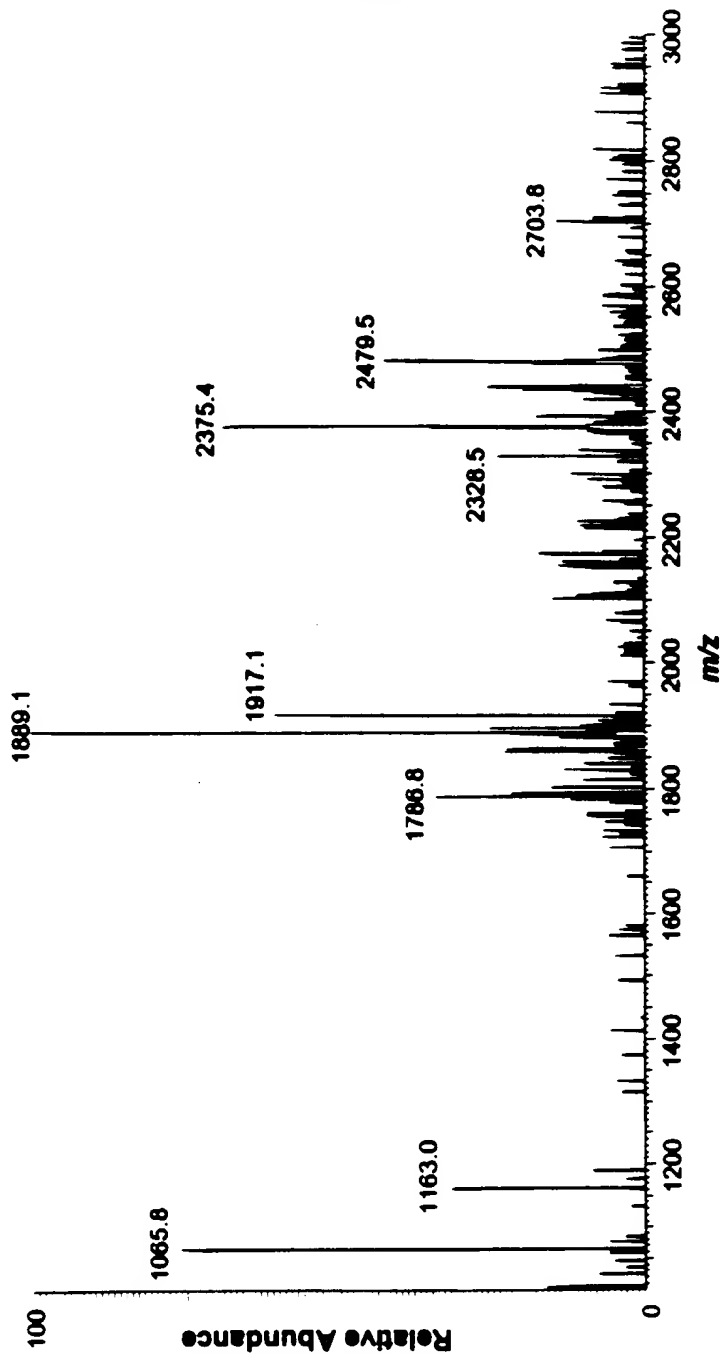


Figure 45

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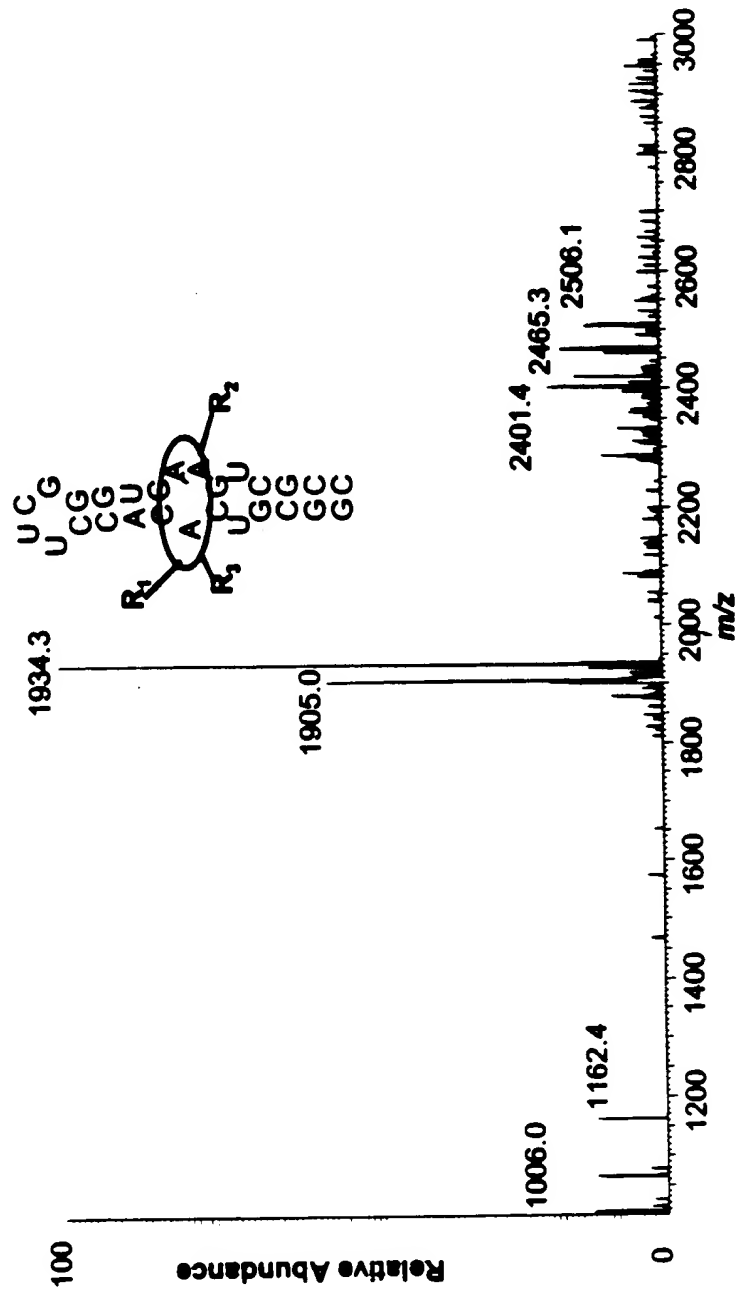


Figure 46